SUPPLEMENTARY MATERIAL

Ligand Efficiency (*LE*), Binding Efficiency Index (*BEI*), and Lipophilic Ligand Efficiency (*LLE*)	
Table S3. Complete results for essential oils from *Valeriana pilosa* with Catalase target: Intermolecular docking energy values ($\Delta E_{binding}$), *Kd* values, Ligand Efficiency (*LE*), Binding Efficiency Index (*BEI*), and Lipophilic Ligand Efficiency (*LLE*)	S11 – S12
Table S4. Complete results for essential oils from *Valeriana pilosa* with Superoxide Dismutase target: Intermolecular docking energy values ($\Delta E_{binding}$), *Kd* values, Ligand Efficiency (*LE*), Binding Efficiency Index (*BEI*), and Lipophilic Ligand Efficiency (*LLE*)	S13 – S14
Table S5. Complete results for essential oils from *Valeriana pilosa* with Xanthine Oxidase target: Intermolecular docking energy values ($\Delta E_{binding}$), *Kd* values, Ligand Efficiency (*LE*), Binding Efficiency Index (*BEI*), and Lipophilic Ligand Efficiency (*LLE*)	S15 – S16
Table S6. mol2 files for all compounds studied in this work.	S16 – S72
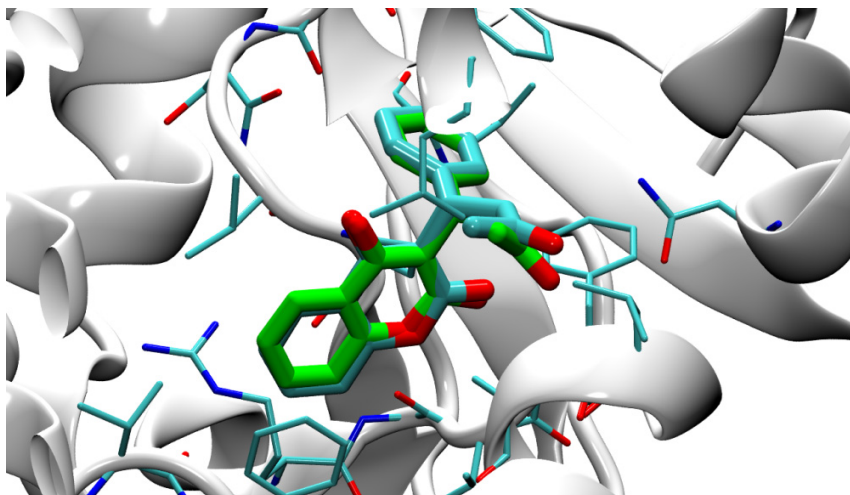
Figure S1. Superposition of the co-crystal warfarine (cyan color) with its docked pose (green color) bound to CYP2C9. Here, complex alignment was performed with respect to ligand and position conformation of the aligned ligands was calculated in terms of RMSD values.
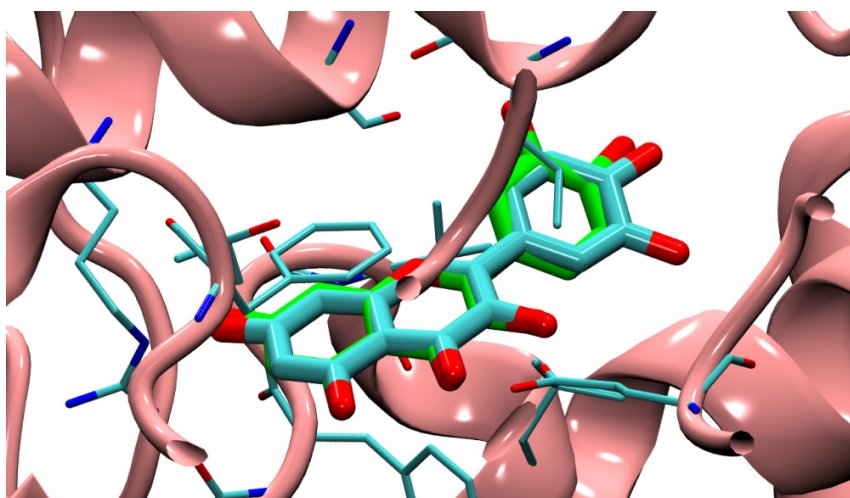
Figure S2. Superposition of the co-crystal quercetin (cyan color) with its docked pose (green color) bound to Xanthine Oxidase. Here, complex alignment was performed with respect to ligand and position conformation of the aligned ligands was calculated in terms of RMSD values.
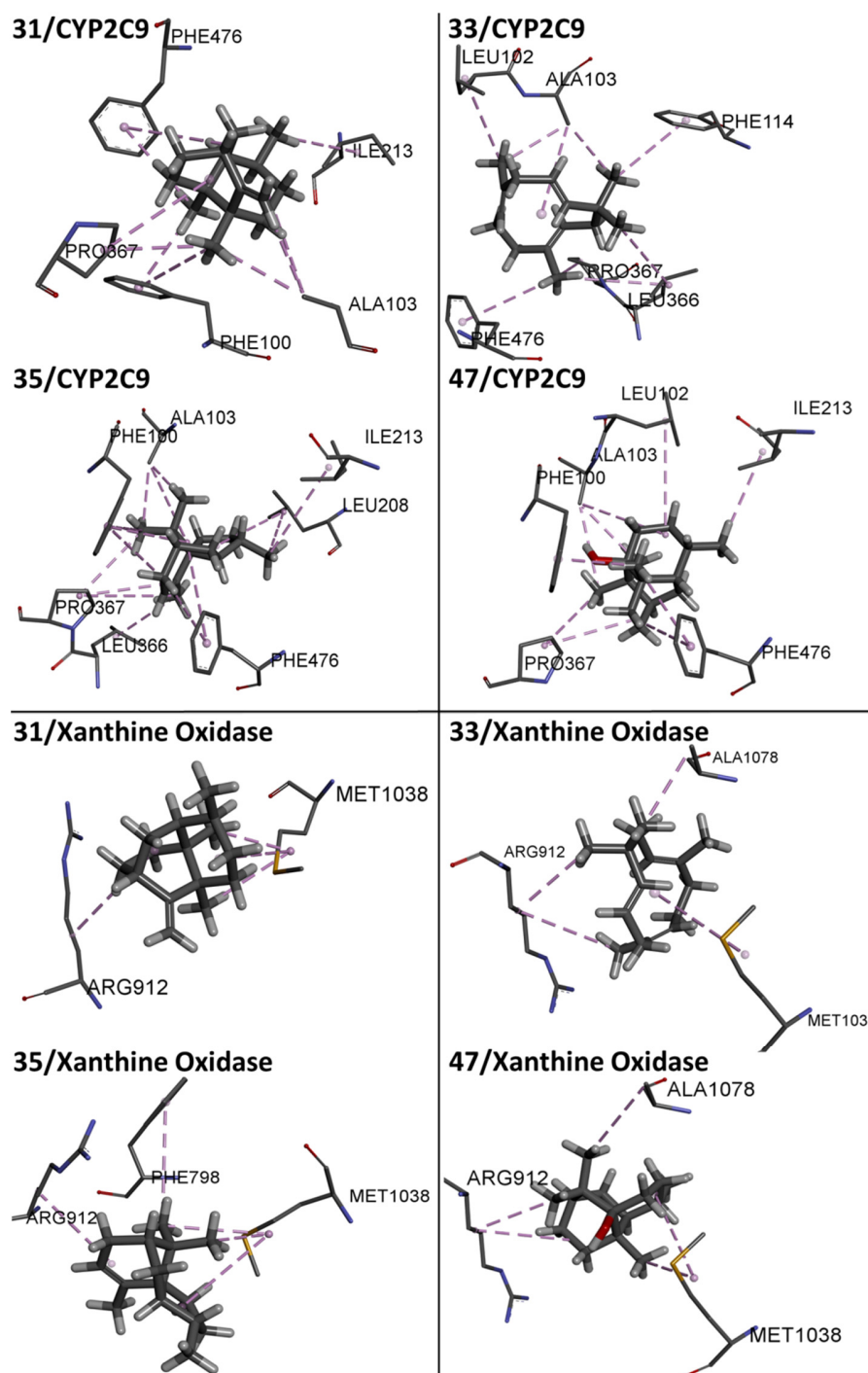
Figure S3. Molecular Docking visualization for the abundant compounds identified in the VPEO bound to CYP2C9 and Xanthine Oxidase.
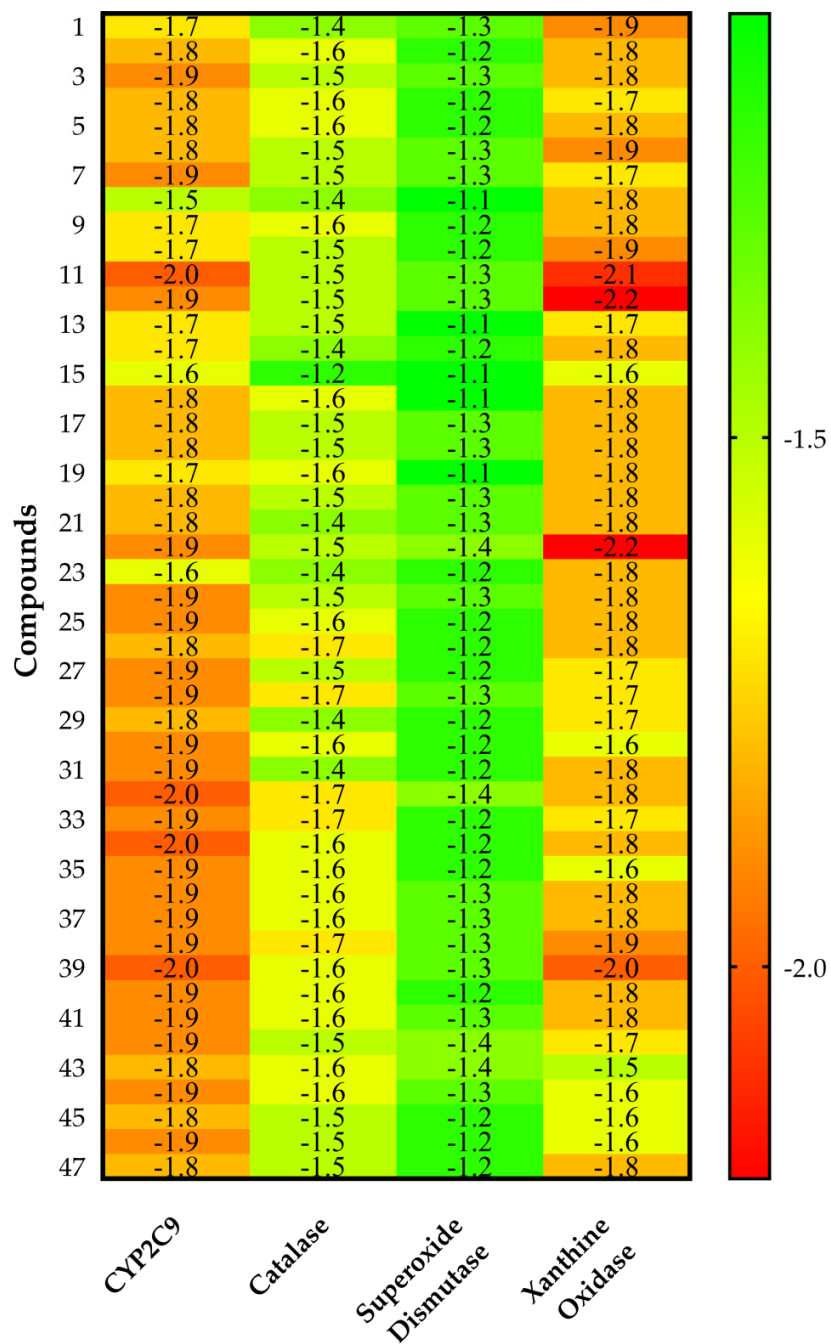
Figure S4. Heat map of the score normalization based on the number of non-Hydrogen Atoms values (kcal·mol⁻¹) of VPEO components.

Table S1. Canonical SMILES of 47 *Valeriana pilosa* essential oils used for ligand efficiency studies.

| N°	Compound Name	Canonical SMILES
1	Isovaleric acid	CC(CC(=O)O)C
2	Tricyclene	C[C@]12[C@@H]3[C@H]1C[C@H](C2(C)C)C3
3	α-Thujene	CC1=CC[C@@]2([C@H]1C2)C(C)C
4	α-Pinene	CC1=CC[C@H]2C[C@@H]1C2(C)C
5	Camphene	C=C1[C@H]2CC[C@@H](C1(C)C)C2
6	3-Methyl valeric acid	C[C@H](CC)CC(=O)O
7	Sabinene	C=C1CC[C@@]2([C@H]1C2)C(C)C
8	1-Octen-3-ol	CCCCC[C@H](C=C)O
9	β-Pinene	C=C1CC[C@H]2C[C@@H]1C2(C)C
10	Myrcene	C=CC(=C)CCC=C(C)C
11	Limonene	CC1=CC[C@@H](CC1)C(=C)C
12	*p*-Cymene	Cc1ccc(cc1)C(C)C
13	1,8-Cineole	C[C@]12CC[C@H](CC1)C(O2)(C)C
14	Linalool	C=C[C@](CCC=C(C)C)(O)C
15	Isopentyl isovalerate	CC(CCOC(=O)CC(C)C)C
16	Camphor	O=C1C[C@H]2C([C@]1(C)CC2)(C)C
17	Menthone	C[C@@H]1CC[C@@H](C(=O)C1)C(C)C
18	Isomenthone	C[C@@H]1CC[C@@H](C(=O)C1)C(C)C
19	Borneol	O[C@@H]1C[C@H]2C([C@]1(C)CC2)(C)C
20	Neomenthol	C[C@H]1CC[C@H]([C@@H](C1)O)C(C)C
21	Menthol	C[C@@H]1CC[C@H]([C@H](C1)O)C(C)C
22	Carvone	CC(=C)[C@@H]1CC=C(C(=O)C1)C
23	Menthyl acetate	C[C@@H]1CC[C@H]([C@@H](C1)OC(=O)C)C(C)C
24	α-Cubebene	CC([C@H]1CC[C@H]([C@@]23[C@@H]1[C@@H]2C(=CC3)C)C)C
25	Cyclosativene	CC([C@H]1CC[C@@H]([C@@]23[C@@H]1[C@@H]1[C@@H]([C@]21C)C3)C)C
26	α-Copaene	C[C@@H]1CC[C@@]2([C@@H]3[C@H]1[C@H]2C(=CC3)C)C
27	β-Patchoulene	C[C@@H]1CCC2=C1C[C@H]1CC[C@@]2(C1(C)C)C
28	β-Bourbonene	CC([C@@H]1CC[C@@]2([C@H]1[C@@H]1C(=C)CC[C@H]21)C)C
29	β-Elemene	C=C[C@@]1(C)CC[C@H](C[C@H]1C(=C)C)C(=C)C
30	β-Caryophyllene	C[C@H]1CCCC(=C)[C@H]2[C@H](CC1)C(C2)(C)C
31	Seychellene	C[C@H]1CC[C@@]2([C@@]3([C@H]1C[C@H](C2=C)CC3)C)C
32	α-Guaiene	CC(=C)[C@@H]1CC[C@@H](C2=C(C1)[C@@H](C)CC2)C
33	α-Humulene	CC1=CCC(C)(C)C=CCC(=CCC1)C
34	allo-Aromadendrene	C[C@H]1CC[C@@H]2[C@H]1[C@@H]1[C@@H](C1(C)C)CCC2=C
35	α-Patchoulene	C[C@H]1CC[C@]23[C@@H]1C[C@@H](C3(C)C)CC=C2C

36	γ-Muurolene	CC1=C[C@H]2[C@@H](CC1)C(=C)CC[C@@H]2C(C)C
37	Germacrene-D	CC1=CCCC(=C)C=C[C@@H](CC1)C(C)C
38	Valencene	CC(=C)[C@@H]1CCC2=CCC[C@H]([C@]2(C1)C)C
39	Eremophyllene	CC(=C)[C@@H]1CC[C@@H]2[C@](C1)(C)C(=CCC2)C
40	γ-Cadinene	CC1=C[C@@H]2[C@H](CC1)C(=C)CC[C@@H]2C(C)C
41	7-epi-α-Selinene	CC1=CCC[C@]2([C@@H]1C[C@@H](CC2)C(=C)C)C
42	δ-Cadinene	CC1=C[C@H]2C(=C(C)CC[C@H]2C(C)C)CC1
43	Spathulenol	C=C1CC[C@H]2[C@@H]([C@@H]3[C@@H]1CC[C@]3(C)O)C2(C)C
44	β-Caryophyllene oxide	C=C1CC[C@@H]2O[C@@]2(CC[C@@H]2[C@@H]1CC2(C)C)C
45	T-Cadinol	CC1=C[C@H]2[C@@H](CC1)[C@@](C)(O)CC[C@H]2C(C)C
46	δ-Cadinol	CC1=C[C@H]2[C@@H](CC1)[C@@](C)(O)CC[C@H]2C(C)C
47	Patchoulol	C[C@H]1CC[C@@]2([C@@]3([C@H]1C[C@H](C2(C)C)CC3)C)O

Table S2. Complete results for essential oils from *Valeriana pilosa* with CYP2C9 target: Intermolecular docking energy values ($\Delta E_{binding}$), K_d values, Ligand Efficiency (*LE*), Binding Efficiency Index (*BEI*), and Lipophilic Ligand Efficiency (*LLE*)

Compound	$\Delta E_{binding}$ (kcal·mol⁻¹)	K_d	LE (kcal·mol⁻¹)	BEI (kDa)	LLE
Isovaleric acid	−4.6	4.25E-04	0.66	33.01	2.25
Tricyclene	−5.8	5.61E-05	0.58	31.20	1.56
α-Thujene	−6.1	3.38E-05	0.61	32.82	1.47
α-Pinene	−5.6	7.87E-05	0.56	30.13	1.11
Camphene	−5.8	5.61E-05	0.58	31.20	1.25
3-Methyl valeric acid	−5.1	1.83E-04	0.64	32.18	2.23
Sabinene	−5.9	4.74E-05	0.59	31.74	1.33
1-Octen-3-ol	−4.5	5.04E-04	0.50	25.72	1.18
β-Pinene	−5.5	9.32E-05	0.55	29.59	1.03
Myrcene	−5.5	9.32E-05	0.55	29.59	0.56
Limonene	−6.2	2.86E-05	0.62	33.35	1.23
p-Cymene	−6.1	3.38E-05	0.61	33.31	1.35
1,8-Cineole	−5.6	7.87E-05	0.51	26.61	1.36
Linalool	−5.6	7.87E-05	0.51	26.61	1.43
Isopentyl isovalerate	−5.5	9.32E-05	0.46	23.40	1.41
Camphor	−6.0	4.01E-05	0.55	28.88	2.00
Menthone	−6.0	4.01E-05	0.55	28.51	1.75
Isomenthone	−6.0	4.01E-05	0.55	28.51	1.75
Borneol	−5.7	6.65E-05	0.52	27.08	1.98
Neomenthol	−6.0	4.01E-05	0.55	28.14	1.96
Menthol	−5.9	4.74E-05	0.54	27.67	1.88
Carvone	−6.4	2.04E-05	0.58	31.22	2.20
Menthyl acetate	−6.1	3.38E-05	0.44	22.54	1.46
α-Cubebene	−7.4	3.77E-06	0.49	26.54	1.15
Cyclosativene	−7.5	3.19E-06	0.50	26.90	1.54
α-Copaene	−6.6	1.46E-05	0.51	27.44	1.20
β-Patchoulene	−7.4	3.77E-06	0.49	26.54	0.86
β-Bourbonene	−7.4	3.77E-06	0.49	26.54	1.15
β-Elemene	−7.0	7.41E-06	0.47	25.10	0.38
β-Caryophyllene	−7.3	4.47E-06	0.49	25.92	0.54
Seychellene	−7.3	4.47E-06	0.49	26.18	0.93
α-Guaiene	−7.7	2.27E-06	0.51	27.61	0.92
α-Humulene	−7.3	4.47E-06	0.49	26.18	0.31
allo-Aromadendrene	−7.6	2.69E-06	0.51	27.26	1.30

α-Patchoulene	−7.3	4.47E-06	0.49	26.18	0.93
γ-Muurolene	−7.4	3.77E-06	0.49	26.54	0.84
Germacrene-D	−7.5	3.19E-06	0.50	26.90	0.61
Valencene	−7.4	3.77E-06	0.49	26.54	0.70
Eremophyllene	−7.8	1.92E-06	0.52	27.97	0.99
γ-Cadinene	−7.5	3.19E-06	0.50	26.90	0.92
7-epi-α-Selinene	−7.3	4.47E-06	0.49	26.18	0.62
δ-Cadinene	−7.4	3.77E-06	0.49	26.54	0.70
Spathulenol	−7.2	5.29E-06	0.45	23.95	1.89
β-Caryophyllene oxide	−7.5	3.19E-06	0.47	24.94	1.56
T-Cadinol	−7.3	4.47E-06	0.46	24.06	1.57
δ-Cadinol	−7.4	3.77E-06	0.46	24.39	1.65
Patchoulol	−7.3	4.47E-06	0.46	24.06	1.74

Table S3. Complete results for essential oils from *Valeriana pilosa* with Catalase target: Intermolecular docking energy values ($\Delta E_{binding}$), K_d values, Ligand Efficiency (*LE*), Binding Efficiency Index (*BEI*), and Lipophilic Ligand Efficiency (*LLE*)

Compound	$\Delta E_{binding}$ (kcal·mol^{-1})	K_d	LE (kcal·mol^{-1})	BEI (kDa)	LLE
Isovaleric acid	−3.7	1.94E-03	0.53	26.55	1.59
Tricyclene	−5.1	1.83E-04	0.51	27.44	1.05
α-Thujene	−4.8	3.04E-04	0.48	25.82	0.52
α-Pinene	−5.0	2.17E-04	0.50	26.90	0.67
Camphene	−5.0	2.17E-04	0.50	26.90	0.67
3-Methyl valeric acid	−4.2	8.35E-04	0.53	26.50	1.57
Sabinene	−4.8	3.04E-04	0.48	25.82	0.52
1-Octen-3-ol	−4.1	9.89E-04	0.46	23.44	0.89
β-Pinene	−5.0	2.17E-04	0.50	26.90	0.67
Myrcene	−4.7	3.59E-04	0.47	25.28	-0.03
Limonene	−4.8	3.04E-04	0.48	25.82	0.21
p-Cymene	−4.8	3.04E-04	0.48	26.21	0.40
1,8-Cineole	−5.0	2.17E-04	0.45	23.76	0.92
Linalool	−4.6	4.25E-04	0.42	21.86	0.70
Isopentyl isovalerate	−4.2	8.35E-04	0.35	17.87	0.46
Camphor	−5.3	1.31E-04	0.48	25.51	1.48
Menthone	−5.1	1.83E-04	0.46	24.23	1.09
Isomenthone	−5.1	1.83E-04	0.46	24.23	1.09
Borneol	−5.2	1.55E-04	0.47	24.71	1.62
Neomenthol	−4.9	2.56E-04	0.45	22.98	1.15
Menthol	−4.8	3.04E-04	0.44	22.51	1.08
Carvone	−5.0	2.17E-04	0.45	24.39	1.18
Menthyl acetate	−5.2	1.55E-04	0.37	19.22	0.80
α-Cubebene	−5.9	4.74E-05	0.39	21.16	0.05
Cyclosativene	−6.2	2.86E-05	0.41	22.24	0.58
α-Copaene	−6.0	4.01E-05	0.46	24.94	0.76
β-Patchoulene	−6.0	4.01E-05	0.40	21.52	-0.16
β-Bourbonene	−6.5	1.72E-05	0.43	23.31	0.49
β-Elemene	−5.6	7.87E-05	0.37	20.08	-0.64
β-Caryophyllene	−6.1	3.38E-05	0.41	21.66	-0.33
Seychellene	−5.6	7.87E-05	0.37	20.08	-0.31
α-Guaiene	−6.4	2.04E-05	0.43	22.95	-0.03
α-Humulene	−6.4	2.04E-05	0.43	22.95	-0.35
allo-Aromadendrene	−6.2	2.86E-05	0.41	22.24	0.27

α-Patchoulene	−6.1	3.38E-05	0.41	21.88	0.06
γ-Muurolene	−6.2	2.86E-05	0.41	22.24	−0.04
Germacrene-D	−6.1	3.38E-05	0.41	21.88	−0.42
Valencene	−6.5	1.72E-05	0.43	23.31	0.04
Eremophyllene	−6.1	3.38E-05	0.41	21.88	−0.25
γ-Cadinene	−6.3	2.41E-05	0.42	22.59	0.04
7-epi-α-Selinene	−6.3	2.41E-05	0.42	22.59	−0.11
δ-Cadinene	−6.0	4.01E-05	0.40	21.52	−0.33
Spathulenol	−6.5	1.72E-05	0.41	21.62	1.38
β-Caryophyllene oxide	−6.5	1.72E-05	0.41	21.62	0.83
T-Cadinol	−5.9	4.74E-05	0.37	19.45	0.55
δ-Cadinol	−5.9	4.74E-05	0.37	19.45	0.55
Patchoulol	−5.9	4.74E-05	0.37	19.45	0.71

Table S4. Complete results for essential oils from *Valeriana pilosa* with Superoxide Dismutase target: Intermolecular docking energy values ($\Delta E_{binding}$), K_d values, Ligand Efficiency (*LE*B), inding Efficiency Index (*BEI*), and Lipophilic Ligand Efficiency (*LLE*)

Compound	$\Delta E_{binding}$ (kcal·mol^{-1})	K_d	LE (kcal·mol^{-1})	BEI (kDa)	LLE
Isovaleric acid	−3.5	2.72E-03	0.50	25.12	1.45
Tricyclene	−3.7	1.94E-03	0.37	19.90	0.02
α-Thujene	−4.1	9.89E-04	0.41	22.06	0.01
α-Pinene	−3.8	1.64E-03	0.38	20.44	−0.21
Camphene	−3.8	1.64E-03	0.38	20.44	−0.21
3-Methyl valeric acid	−3.7	1.94E-03	0.46	23.34	1.20
Sabinene	−4.1	9.89E-04	0.41	22.06	0.01
1-Octen-3-ol	−3.4	3.22E-03	0.38	19.43	0.38
β-Pinene	−3.8	1.64E-03	0.38	20.44	−0.21
Myrcene	−3.7	1.94E-03	0.37	19.90	−0.76
Limonene	−4.2	8.35E-04	0.42	22.59	−0.23
p-Cymene	−4.1	9.89E-04	0.41	22.39	−0.11
1,8-Cineole	−3.8	1.64E-03	0.35	18.05	0.04
Linalool	−3.9	1.39E-03	0.35	18.53	0.19
Isopentyl isovalerate	−3.9	1.39E-03	0.33	16.59	0.24
Camphor	−3.8	1.64E-03	0.35	18.29	0.38
Menthone	−4.2	8.35E-04	0.38	19.96	0.43
Isomenthone	−4.2	8.35E-04	0.38	19.96	0.43
Borneol	−3.8	1.64E-03	0.35	18.05	0.59
Neomenthol	−4.2	8.35E-04	0.38	19.70	0.64
Menthol	−4.3	7.06E-04	0.39	20.17	0.71
Carvone	−4.7	3.59E-04	0.43	22.93	0.96
Menthyl acetate	−4.6	4.25E-04	0.33	17.00	0.36
α-Cubebene	−5.0	2.17E-04	0.33	17.93	−0.61
Cyclosativene	−4.8	3.04E-04	0.32	17.21	−0.44
α-Copaene	−4.5	5.04E-04	0.35	18.71	−0.34
β-Patchoulene	−4.8	3.04E-04	0.32	17.21	−1.04

β-Bourbonene	−5.2	1.55E-04	0.35	18.65	−0.46
β-Elemene	−4.6	4.25E-04	0.31	16.50	−1.38
β-Caryophyllene	−4.7	3.59E-04	0.31	16.69	−1.36
Seychellene	−4.7	3.59E-04	0.31	16.86	−0.97
α-Guaiene	−5.5	9.32E-05	0.37	19.72	−0.69
α-Humulene	−4.6	4.25E-04	0.31	16.50	−1.66
allo-Aromadendrene	−4.8	3.04E-04	0.32	17.21	−0.75
α-Patchoulene	−4.5	5.04E-04	0.30	16.14	−1.12
γ-Muurolene	−5.2	1.55E-04	0.35	18.65	−0.77
Germacrene-D	−4.9	2.56E-04	0.33	17.57	−1.30
Valencene	−5.0	2.17E-04	0.33	17.93	−1.06
Eremophyllene	−5.1	1.83E-04	0.34	18.29	−0.99
γ-Cadinene	−4.8	3.04E-04	0.32	17.21	−1.06
7-epi-α-Selinene	−5.0	2.17E-04	0.33	17.93	−1.06
δ-Cadinene	−5.5	9.32E-05	0.37	19.72	−0.69
Spathulenol	−5.5	9.32E-05	0.34	18.29	0.64
β-Caryophyllene oxide	−5.2	1.55E-04	0.33	17.29	−0.13
T-Cadinol	−4.8	3.04E-04	0.30	15.82	−0.26
δ-Cadinol	−4.8	3.04E-04	0.30	15.82	−0.26
Patchoulol	−4.7	3.59E-04	0.29	15.49	−0.17

Table S5. Complete results for essential oils from *Valeriana pilosa* with Xanthine Oxidase target: Intermolecular docking energy values ($\Delta E_{binding}$), K_d values, Ligand Efficiency (*LE*), Binding Efficiency Index (*BEI*), and Lipophilic Ligand Efficiency (*LLE*)

Compound	$\Delta E_{binding}$ (kcal·mol⁻¹)	K_d	LE (kcal·mol⁻¹)	BEI (kDa)	LLE
Isovaleric acid	−5.0	2.17E-04	0.71	35.88	2.55
Tricyclene	−5.6	7.87E-05	0.56	30.13	1.42
α-Thujene	−5.6	7.87E-05	0.56	30.13	1.11
α-Pinene	−5.5	9.32E-05	0.55	29.59	1.03
Camphene	−5.7	6.65E-05	0.57	30.66	1.18
3-Methyl valeric acid	−5.3	1.31E-04	0.66	33.44	2.38
Sabinene	−5.5	9.32E-05	0.55	29.59	1.03
1-Octen-3-ol	−5.4	1.10E-04	0.60	30.87	1.84
β-Pinene	−5.6	7.87E-05	0.56	30.13	1.11
Myrcene	−6.1	3.38E-05	0.61	32.82	1.00
Limonene	−6.7	1.23E-05	0.67	36.04	1.60
p-Cymene	−7.0	7.41E-06	0.70	38.22	2.01
1,8-Cineole	−5.7	6.65E-05	0.52	27.08	1.43
Linalool	−6.0	4.01E-05	0.55	28.51	1.73
Isopentyl isovalerate	−5.6	7.87E-05	0.47	23.82	1.48
Camphor	−6.1	3.38E-05	0.55	29.37	2.07
Menthone	−6.1	3.38E-05	0.55	28.98	1.82
Isomenthone	−6.1	3.38E-05	0.55	28.98	1.82
Borneol	−6.0	4.01E-05	0.55	28.51	2.20
Neomenthol	−6.1	3.38E-05	0.55	28.61	2.03
Menthol	−5.9	4.74E-05	0.54	27.67	1.88
Carvone	−7.2	5.29E-06	0.65	35.13	2.79
Menthyl acetate	−6.6	1.46E-05	0.47	24.39	1.83
α-Cubebene	−7.0	7.41E-06	0.47	25.10	0.86
Cyclosativene	−7.0	7.41E-06	0.47	25.10	1.17
α-Copaene	−6.6	1.46E-05	0.51	27.44	1.20

β-Patchoulene	−6.6	1.46E-05	0.44	23.67	0.28
β-Bourbonene	−6.6	1.46E-05	0.44	23.67	0.57
β-Elemene	−6.5	1.72E-05	0.43	23.31	0.02
β-Caryophyllene	−6.1	3.38E-05	0.41	21.66	−0.33
Seychellene	−6.8	1.04E-05	0.45	24.39	0.57
α-Guaiene	−7.0	7.41E-06	0.47	25.10	0.40
α-Humulene	−6.5	1.72E-05	0.43	23.31	−0.27
allo-Aromadendrene	−7.0	7.41E-06	0.47	25.10	0.86
α-Patchoulene	−6.2	2.86E-05	0.41	22.24	0.13
γ-Muurolene	−6.9	8.77E-06	0.46	24.75	0.48
Germacrene-D	−6.8	1.04E-05	0.45	24.39	0.09
Valencene	−7.3	4.47E-06	0.49	26.18	0.62
Eremophyllene	−7.6	2.69E-06	0.51	27.26	0.84
γ-Cadinene	−6.8	1.04E-05	0.45	24.39	0.40
7-epi-α-Selinene	−7.1	6.26E-06	0.47	25.46	0.48
δ-Cadinene	−6.5	1.72E-05	0.43	23.31	0.04
Spathulenol	−6.1	3.38E-05	0.38	20.29	1.08
β-Caryophyllene oxide	−6.5	1.72E-05	0.41	21.62	0.83
T-Cadinol	−6.3	2.41E-05	0.39	20.76	0.84
δ-Cadinol	−6.3	2.41E-05	0.39	20.76	0.84
Patchoulol	−7.0	7.41E-06	0.44	23.07	1.52

Table S6. .mol2 files for all compounds studied in this work.

Compound 1
@<TRIPOS>MOLECULE
compuesto_1.out
17 16 0 0 0
SMALL
MULLIKEN_CHARGES
@<TRIPOS>ATOM
1 C   -11.9915   0.7844   0.2482 C.3   1 UNL1   -0.5082
2 C   -10.7395 -0.1045   0.3425 C.3   1 UNL1   0.0630
3 C   -9.4784   0.7163 -0.0274 C.3   1 UNL1   -0.4278
4 C   -8.1768 -0.0237   0.1933 C.2   1 UNL1   0.6395
5 O   -7.1808   0.5141 -0.5653 O.3   1 UNL1   -0.5153
6 C   -10.8939 -1.3344 -0.5708 C.3   1 UNL1   -0.5064
7 O   -7.9583 -0.9609   0.9228 O.2   1 UNL1   -0.5200
8 H   -11.9483   1.6438   0.9599 H   1 UNL1   0.1533
9 H   -12.1443   1.1612 -0.7794 H   1 UNL1   0.1557
10 H   -12.9034   0.2139   0.5123 H   1 UNL1   0.1577
11 H   -10.6382 -0.4536   1.3980 H   1 UNL1   0.1265
12 H   -9.5728   1.0315 -1.0862 H   1 UNL1   0.1896
13 H   -9.4255   1.6480   0.5912 H   1 UNL1   0.1859
14 H   -6.3578   0.0111 -0.3942 H   1 UNL1   0.3337
15 H   -11.7979 -1.9264 -0.2844 H   1 UNL1   0.1583
16 H   -11.0005 -1.0392 -1.6312 H   1 UNL1   0.1516
17 H   -10.0080 -1.9956 -0.5194 H   1 UNL1   0.1628
@<TRIPOS>BOND
1 16   6 1
2 12   3 1
3   9   1 1
4   6 17 1
5   6 15 1
6   6   2 1
7   5 14 1
8   5   4 1
9   3   4 1
10   3   2 1
11   3 13 1
12   4   7 2
13   1   2 1
14   1 10 1
15   1   8 1
16   2 11 1

Compound 2
@<TRIPOS>MOLECULE
compuesto_2.out
26 28 0 0 0
SMALL
MULLIKEN_CHARGES
@<TRIPOS>ATOM
1 C   -10.1093   0.8568   0.4249 C.3   1 UNL1   -0.1864
2 C   -10.5753 -0.5750   0.1219 C.3   1 UNL1   -0.2730
3 C   -9.3919 -0.9748 -0.8188 C.3   1 UNL1   -0.1189
4 C   -8.1257 -0.6046   0.0610 C.3   1 UNL1   0.1815
5 C   -8.5666   0.8584   0.3809 C.3   1 UNL1   0.0104
6 C   -9.3773   1.3508 -0.8388 C.3   1 UNL1   -0.1862
7 C   -9.4367   0.1966 -1.8517 C.3   1 UNL1   -0.2726
8 C   -7.7263   1.7576   1.2218 C.3   1 UNL1   -0.4703
9 C   -6.8189 -0.6776 -0.7293 C.3   1 UNL1   -0.5159
10 C   -8.0014 -1.4769   1.3113 C.3   1 UNL1   -0.5161
11 H   -10.6946   1.4837   1.0734 H   1 UNL1   0.1445

12 H	-10.6469	-1.2042	1.0172 H	1	UNL1	0.1352
13 H	-11.5514	-0.6040	-0.3801 H	1	UNL1	0.1347
14 H	-9.4122	-1.9831	-1.2236 H	1	UNL1	0.1242
15 H	-9.3854	2.3678	-1.1855 H	1	UNL1	0.1443
16 H	-10.3622	0.2056	-2.4432 H	1	UNL1	0.1347
17 H	-8.5993	0.1924	-2.5599 H	1	UNL1	0.1351
18 H	-7.5566	1.3299	2.2177 H	1	UNL1	0.1574
19 H	-6.7411	1.9254	0.7694 H	1	UNL1	0.1571
20 H	-8.1921	2.7408	1.3604 H	1	UNL1	0.1528
21 H	-6.7844	0.0598	-1.5396 H	1	UNL1	0.1585
22 H	-5.9554	-0.4826	-0.0846 H	1	UNL1	0.1530
23 H	-6.6853	-1.6703	-1.1713 H	1	UNL1	0.1523
24 H	-8.8290	-1.3156	2.0112 H	1	UNL1	0.1585
25 H	-7.9886	-2.5404	1.0522 H	1	UNL1	0.1520
26 H	-7.0718	-1.2597	1.8491 H	1	UNL1	0.1532

@<TRIPOS>BOND

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 1   17   7   1
 2   16   7   1
 3    7   6   1
 4    7   3   1
 5   21   9   1
 6   14   3   1
 7   15   6   1
 8   23   9   1
 9    6   5   1
10    6   1   1
11    3   4   1
12    3   2   1
13    9  22   1
14    9   4   1
15   13   2   1
16    4   5   1
17    4  10   1
18    2   1   1
19    2  12   1
20    5   1   1
21    5   8   1
22    1  11   1
23   19   8   1
24   25  10   1
25    8  20   1
26    8  18   1
27   10  26   1
28   10  24   1
```

Compound 3

@<TRIPOS>MOLECULE
compuesto_3.out
 26 27 0 0 0
SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM

1 C	-8.6021	0.3558	-5.4823 C.3	1	UNL1	0.0319
2 C	-8.0494	-1.0659	-5.2292 C.3	1	UNL1	-0.2026
3 C	-8.7184	-0.2830	-4.1032 C.3	1	UNL1	-0.3555
4 C	-9.8269	0.1762	-6.4004 C.3	1	UNL1	-0.2675
5 C	-9.9559	-1.3235	-6.5783 C.2	1	UNL1	-0.2511
6 C	-8.9726	-2.0031	-5.9569 C.2	1	UNL1	0.0926
7 C	-8.7793	-3.4700	-5.8888 C.3	1	UNL1	-0.4903
8 C	-7.7553	1.6014	-5.7079 C.3	1	UNL1	-0.0004
9 C	-8.5069	2.8192	-5.1573 C.3	1	UNL1	-0.4893
10 C	-6.3653	1.5076	-5.0642 C.3	1	UNL1	-0.4909
11 H	-6.9963	-1.3109	-5.1913 H	1	UNL1	0.1538
12 H	-9.6919	-0.6071	-3.7417 H	1	UNL1	0.1605
13 H	-8.1106	0.0941	-3.2871 H	1	UNL1	0.1540

14 H	-10.7379	0.6105	-5.9536 H	1	UNL1	0.1455	
15 H	-9.6766	0.6768	-7.3718 H	1	UNL1	0.1438	
16 H	-10.7763	-1.7340	-7.1370 H	1	UNL1	0.1486	
17 H	-9.5657	-4.0209	-6.4228 H	1	UNL1	0.1603	
18 H	-7.8178	-3.7783	-6.3200 H	1	UNL1	0.1644	
19 H	-8.7946	-3.8198	-4.8417 H	1	UNL1	0.1671	
20 H	-7.6154	1.7263	-6.8137 H	1	UNL1	0.1207	
21 H	-7.9455	3.7437	-5.3231 H	1	UNL1	0.1476	
22 H	-9.4890	2.9353	-5.6267 H	1	UNL1	0.1492	
23 H	-8.6730	2.7246	-4.0774 H	1	UNL1	0.1550	
24 H	-5.7898	2.4246	-5.2405 H	1	UNL1	0.1495	
25 H	-6.4303	1.3664	-3.9791 H	1	UNL1	0.1527	
26 H	-5.7816	0.6745	-5.4680 H	1	UNL1	0.1503	

@<TRIPOS>BOND
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 1   15   4   1
 2   16   5   1
 3   20   8   1
 4    5   4   1
 5    5   6   2
 6   17   7   1
 7    4  14   1
 8    4   1   1
 9   18   7   1
10    6   7   1
11    6   2   1
12    7  19   1
13    8   1   1
14    8   9   1
15    8  10   1
16   22   9   1
17    1   2   1
18    1   3   1
19   26  10   1
20   21   9   1
21   24  10   1
22    2  11   1
23    2   3   1
24    9  23   1
25   10  25   1
26    3  12   1
27    3  13   1
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Compound 4

@<TRIPOS>MOLECULE
compuesto_4.out
 26 27 0 0 0
SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM

1 C	-10.1088	0.8924	-5.9739 C.3	1	UNL1	-0.1658	
2 C	-10.3430	-0.5394	-6.6127 C.3	1	UNL1	0.1866	
3 C	-9.7164	-1.0831	-5.2653 C.3	1	UNL1	-0.1235	
4 C	-8.1766	-1.0078	-5.3088 C.3	1	UNL1	-0.2545	
5 C	-7.7292	0.3434	-5.8245 C.2	1	UNL1	-0.2406	
6 C	-8.6499	1.2731	-6.1472 C.2	1	UNL1	0.0767	
7 C	-10.2343	0.2148	-4.5709 C.3	1	UNL1	-0.3041	
8 C	-11.8284	-0.8898	-6.7259 C.3	1	UNL1	-0.5242	
9 C	-9.6353	-0.8699	-7.9177 C.3	1	UNL1	-0.5175	
10 C	-8.3444	2.6356	-6.6623 C.3	1	UNL1	-0.4981	
11 H	-10.8268	1.6743	-6.2270 H	1	UNL1	0.1324	
12 H	-10.0925	-2.0403	-4.8989 H	1	UNL1	0.1219	
13 H	-7.7625	-1.1735	-4.2946 H	1	UNL1	0.1358	
14 H	-7.7649	-1.8164	-5.9393 H	1	UNL1	0.1354	
15 H	-6.6618	0.4867	-5.9166 H	1	UNL1	0.1414	
16 H	-9.5999	0.6335	-3.7867 H	1	UNL1	0.1425	

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    17 H    -11.2570   0.1518  -4.1899 H    1 UNL1    0.1324
    18 H    -12.4292  -0.4162  -5.9419 H    1 UNL1    0.1552
    19 H    -12.2455  -0.5616  -7.6843 H    1 UNL1    0.1545
    20 H    -11.9757  -1.9728  -6.6538 H    1 UNL1    0.1557
    21 H     -9.0985  -1.8221  -7.8456 H    1 UNL1    0.1564
    22 H    -10.3291  -0.9480  -8.7613 H    1 UNL1    0.1506
    23 H     -8.9040  -0.1035  -8.1965 H    1 UNL1    0.1654
    24 H     -7.3166   2.7276  -7.0361 H    1 UNL1    0.1592
    25 H     -9.0231   2.9150  -7.4796 H    1 UNL1    0.1618
    26 H     -8.4729   3.3893  -5.8724 H    1 UNL1    0.1644
@<TRIPOS>BOND
    1   22    9   1
    2   23    9   1
    3    9   21   1
    4    9    2   1
    5   19    8   1
    6   25   10   1
    7   24   10   1
    8    8   20   1
    9    8    2   1
   10    8   18   1
   11   10    6   1
   12   10   26   1
   13    2    1   1
   14    2    3   1
   15   11    1   1
   16    6    1   1
   17    6    5   2
   18    1    7   1
   19   14    4   1
   20   15    5   1
   21    5    4   1
   22    4    3   1
   23    4   13   1
   24    3   12   1
   25    3    7   1
   26    7   17   1
   27    7   16   1
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Compound 5

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@<TRIPOS>MOLECULE
compuesto_5.out
 26 27 0 0 0
SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM
     1 C     -9.2218  -0.0323  -7.1842 C.3    1 UNL1   -0.2753
     2 C     -9.5794  -0.4504  -5.7329 C.3    1 UNL1   -0.1015
     3 C     -8.2625  -0.8132  -4.9451 C.3    1 UNL1    0.1549
     4 C     -7.5910   0.5695  -4.8322 C.2    1 UNL1    0.0488
     5 C     -8.4978   1.3314  -7.0003 C.3    1 UNL1   -0.2668
     6 C     -8.5582   1.5680  -5.4613 C.3    1 UNL1   -0.0927
     7 C     -9.9351   0.9320  -5.1073 C.3    1 UNL1   -0.3052
     8 C     -8.6299  -1.3371  -3.5480 C.3    1 UNL1   -0.5113
     9 C     -7.3848  -1.8339  -5.6800 C.3    1 UNL1   -0.5075
    10 C     -6.4134   0.8478  -4.2826 C.2    1 UNL1   -0.4329
    11 H     -8.5758  -0.7625  -7.6900 H      1 UNL1    0.1336
    12 H    -10.1276   0.0653  -7.8015 H      1 UNL1    0.1276
    13 H    -10.3509  -1.2231  -5.6618 H      1 UNL1    0.1215
    14 H     -9.0037   2.1414  -7.5445 H      1 UNL1    0.1286
    15 H     -7.4577   1.2862  -7.3589 H      1 UNL1    0.1343
    16 H     -8.4194   2.6109  -5.1560 H      1 UNL1    0.1271
    17 H    -10.1475   0.8923  -4.0339 H      1 UNL1    0.1362
    18 H    -10.7805   1.4360  -5.5888 H      1 UNL1    0.1371
    19 H     -9.0988  -0.5567  -2.9347 H      1 UNL1    0.1568
```

20 H	-9.3324	-2.1719	-3.6252 H	1 UNL1	0.1521		
21 H	-7.7485	-1.6908	-3.0009 H	1 UNL1	0.1554		
22 H	-6.7190	-1.3450	-6.4064 H	1 UNL1	0.1590		
23 H	-6.7434	-2.3867	-4.9844 H	1 UNL1	0.1537		
24 H	-7.9890	-2.5725	-6.2218 H	1 UNL1	0.1530		
25 H	-5.9955	1.8392	-4.2277 H	1 UNL1	0.1554		
26 H	-5.7694	0.0925	-3.8512 H	1 UNL1	0.1581		

@<TRIPOS>BOND

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 2   11    1   1
 3   14    5   1
 4   15    5   1
 5    1    5   1
 6    1    2   1
 7    5    6   1
 8   22    9   1
 9   24    9   1
10    2   13   1
11    2    7   1
12    2    3   1
13    9   23   1
14    9    3   1
15   18    7   1
16    6   16   1
17    6    7   1
18    6    4   1
19    7   17   1
20    3    4   1
21    3    8   1
22    4   10   2
23   10   25   1
24   10   26   1
25   20    8   1
26    8   21   1
27    8   19   1
```

Compound 6

@<TRIPOS>MOLECULE
compuesto_6.out
 20 19 0 0 0
SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM

1 C	-6.8697	0.7602	-8.9193 C.3	1 UNL1	-0.2665
2 C	-6.2783	-0.1072	-7.7830 C.3	1 UNL1	0.0216
3 C	-5.2969	0.7401	-6.9274 C.3	1 UNL1	-0.4310
4 C	-4.8102	0.0533	-5.6780 C.2	1 UNL1	0.6417
5 O	-3.6247	0.5788	-5.2592 O.3	1 UNL1	-0.5155
6 C	-5.5720	-1.3590	-8.3258 C.3	1 UNL1	-0.4962
7 O	-5.3403	-0.8414	-5.0554 O.2	1 UNL1	-0.5218
8 C	-7.9589	0.0555	-9.7322 C.3	1 UNL1	-0.4490
9 H	-7.3110	1.6822	-8.4841 H	1 UNL1	0.1298
10 H	-6.0451	1.1009	-9.5804 H	1 UNL1	0.1337
11 H	-7.1221	-0.4252	-7.1221 H	1 UNL1	0.1320
12 H	-4.4338	1.0281	-7.5664 H	1 UNL1	0.1898
13 H	-5.7759	1.6814	-6.5966 H	1 UNL1	0.1833
14 H	-3.3475	0.1058	-4.4421 H	1 UNL1	0.3355
15 H	-5.1221	-1.9490	-7.5235 H	1 UNL1	0.1586
16 H	-6.2824	-2.0330	-8.8377 H	1 UNL1	0.1582
17 H	-4.7685	-1.0678	-9.0382 H	1 UNL1	0.1524
18 H	-7.5628	-0.7973	-10.3124 H	1 UNL1	0.1493
19 H	-8.7680	-0.3188	-9.0780 H	1 UNL1	0.1494
20 H	-8.4099	0.7550	-10.4571 H	1 UNL1	0.1447

@<TRIPOS>BOND

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 1   20    8   1
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2	18	8	1
3	8	19	1
4	8	1	1
5	10	1	1
6	17	6	1
7	1	9	1
8	1	2	1
9	16	6	1
10	6	2	1
11	6	15	1
12	2	11	1
13	2	3	1
14	12	3	1
15	3	13	1
16	3	4	1
17	4	5	1
18	4	7	2
19	5	14	1

Compound 7

@<TRIPOS>MOLECULE
compuesto_7.out
 26 27 0 0 0
SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM
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    1 C      -7.2629   0.2711  -9.1354 C.3    1 UNL1      0.0352
    2 C      -6.8701  -1.1366  -8.6363 C.3    1 UNL1     -0.2148
    3 C      -7.8943  -0.3015  -7.8769 C.3    1 UNL1     -0.3478
    4 C      -8.0658   0.0888 -10.4293 C.3    1 UNL1     -0.2722
    5 C      -8.3819  -1.4228 -10.5351 C.3    1 UNL1     -0.3072
    6 C      -7.4076  -2.1314  -9.6125 C.2    1 UNL1      0.1536
    7 C      -7.0500  -3.4106  -9.6941 C.2    1 UNL1     -0.4658
    8 C      -6.3870   1.5158  -9.0840 C.3    1 UNL1     -0.0018
    9 C      -7.2640   2.7545  -8.8527 C.3    1 UNL1     -0.4886
   10 C      -5.2980   1.4174  -8.0084 C.3    1 UNL1     -0.4919
   11 H      -5.9069  -1.3455  -8.1785 H      1 UNL1      0.1591
   12 H      -8.9407  -0.5954  -7.8757 H      1 UNL1      0.1594
   13 H      -7.6180   0.1106  -6.9124 H      1 UNL1      0.1555
   14 H      -8.9716   0.7133 -10.4261 H      1 UNL1      0.1386
   15 H      -7.4678   0.4136 -11.2995 H      1 UNL1      0.1393
   16 H      -8.2912  -1.7781 -11.5749 H      1 UNL1      0.1471
   17 H      -9.4179  -1.6388 -10.2064 H      1 UNL1      0.1502
   18 H      -6.3600  -3.8787  -9.0115 H      1 UNL1      0.1634
   19 H      -7.4201  -4.0886 -10.4445 H      1 UNL1      0.1607
   20 H      -5.8754   1.6210 -10.0782 H      1 UNL1      0.1206
   21 H      -6.6681   3.6731  -8.8338 H      1 UNL1      0.1488
   22 H      -8.0113   2.8690  -9.6447 H      1 UNL1      0.1483
   23 H      -7.8063   2.6900  -7.9018 H      1 UNL1      0.1553
   24 H      -4.6882   2.3261  -7.9767 H      1 UNL1      0.1502
   25 H      -5.7267   1.2807  -7.0095 H      1 UNL1      0.1532
   26 H      -4.6222   0.5760  -8.1968 H      1 UNL1      0.1517
```
@<TRIPOS>BOND
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    2   15    4  1
    3    5    4  1
    4    5   17  1
    5    5    6  1
    6   19    7  1
    7    4   14  1
    8    4    1  1
    9   20    8  1
   10    7    6  2
   11    7   18  1
   12   22    9  1
```

13	6	2	1
14	1	8	1
15	1	2	1
16	1	3	1
17	8	9	1
18	8	10	1
19	9	21	1
20	9	23	1
21	2	11	1
22	2	3	1
23	26	10	1
24	10	24	1
25	10	25	1
26	3	12	1
27	3	13	1

Compound 8

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compuesto_8.out
 25 24 0 0 0
SMALL
MULLIKEN_CHARGES

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      1 O    -9.4109   0.9451 -12.0316 O.3   1 UNL1   -0.5625
      2 H    -3.8677   1.0715  -6.7700 H     1 UNL1    0.1470
      3 H    -5.1830   1.7052  -5.7575 H     1 UNL1    0.1475
      4 H    -6.6122  -0.2993  -6.3315 H     1 UNL1    0.1265
      5 H    -5.3062  -0.9461  -7.3674 H     1 UNL1    0.1269
      6 H    -6.7630   1.7504  -7.7971 H     1 UNL1    0.1351
      7 H    -5.4579   1.1033  -8.8337 H     1 UNL1    0.1345
      8 H    -8.1847  -0.2628  -8.3492 H     1 UNL1    0.1326
      9 H    -6.8783  -0.9133  -9.3787 H     1 UNL1    0.1359
     10 H    -8.2967   1.7977  -9.8110 H     1 UNL1    0.1578
     11 H    -7.0209   1.1385 -10.8563 H     1 UNL1    0.1556
     12 H    -9.7903  -0.1572 -10.3508 H     1 UNL1    0.1097
     13 H    -9.9068   0.3882 -12.6656 H     1 UNL1    0.3118
     14 C    -9.0786  -2.2884 -11.7630 C.2   1 UNL1   -0.3212
     15 C    -8.3715  -1.1602 -11.6594 C.2   1 UNL1   -0.1967
     16 C    -4.7424   0.7798  -6.1685 C.3   1 UNL1   -0.4635
     17 C    -5.7687  -0.0077  -6.9910 C.3   1 UNL1   -0.2218
     18 C    -6.3036   0.8125  -8.1786 C.3   1 UNL1   -0.2667
     19 C    -7.3362   0.0262  -9.0040 C.3   1 UNL1   -0.2548
     20 C    -7.8610   0.8522 -10.1914 C.3   1 UNL1   -0.3167
     21 C    -8.9128   0.0810 -10.9928 C.3   1 UNL1    0.1756
     22 H    -4.3771   0.1733  -5.3236 H     1 UNL1    0.1449
     23 H    -7.3691  -1.0705 -12.0840 H     1 UNL1    0.1576
     24 H    -8.6697  -3.1664 -12.2427 H     1 UNL1    0.1535
     25 H   -10.0866  -2.3990 -11.3775 H     1 UNL1    0.1514
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    2   24   14   1
    3   23   15   1
    4    1   21   1
    5   14   15   2
    6   14   25   1
    7   15   21   1
    8   21   12   1
    9   21   20   1
   10   11   20   1
   11   20   10   1
   12   20   19   1
   13    9   19   1
   14   19    8   1
   15   19   18   1
   16    7   18   1
```

17	18	6	1
18	18	17	1
19	5	17	1
20	17	4	1
21	17	16	1
22	2	16	1
23	16	3	1
24	16	22	1

Compound 9

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@<TRIPOS>MOLECULE
compuesto_9.out
 26 27 0 0 0
SMALL
MULLIKEN_CHARGES

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   1 C    -9.0296   0.9557 -10.7318 C.3   1 UNL1   -0.1793
   2 H    -6.3090   3.1143 -10.2393 H     1 UNL1    0.1590
   3 H    -7.8881   3.4767 -11.0141 H     1 UNL1    0.1616
   4 H    -7.3919   0.2133 -12.7450 H     1 UNL1    0.1627
   5 H    -7.9459  -1.4226 -13.1051 H     1 UNL1    0.1524
   6 H    -6.8610  -1.1689 -11.7596 H     1 UNL1    0.1595
   7 H   -10.4095  -2.0017 -11.7966 H     1 UNL1    0.1556
   8 H   -10.1376  -0.8898 -13.1552 H     1 UNL1    0.1563
   9 H   -11.0759  -0.3674 -11.7642 H     1 UNL1    0.1555
  10 H   -10.7252   0.1900  -9.4708 H     1 UNL1    0.1348
  11 H    -9.3574   0.7457  -8.5034 H     1 UNL1    0.1429
  12 H    -5.8842   0.2803 -10.2892 H     1 UNL1    0.1458
  13 H    -6.3592   0.9064  -8.7087 H     1 UNL1    0.1441
  14 H    -6.8138  -1.7253  -9.6952 H     1 UNL1    0.1290
  15 H    -7.4727  -1.0360  -8.2066 H     1 UNL1    0.1307
  16 H    -9.3385  -1.9486  -9.6758 H     1 UNL1    0.1227
  17 H    -9.6472   1.6827 -11.2684 H     1 UNL1    0.1384
  18 C    -7.2714   2.7302 -10.5378 C.2   1 UNL1   -0.4862
  19 C    -7.7162  -0.7302 -12.2881 C.3   1 UNL1   -0.5192
  20 C   -10.1981  -0.9551 -12.0608 C.3   1 UNL1   -0.5238
  21 C    -9.6357   0.2926  -9.4583 C.3   1 UNL1   -0.3020
  22 C    -7.6641   1.4689 -10.3334 C.2   1 UNL1    0.1526
  23 C    -6.7655   0.4611  -9.6399 C.3   1 UNL1   -0.3030
  24 C    -7.4351  -0.8981  -9.3044 C.3   1 UNL1   -0.2578
  25 C    -8.8540  -0.9889  -9.8766 C.3   1 UNL1   -0.1225
  26 C    -8.9094  -0.4848 -11.3739 C.3   1 UNL1    0.1903
@<TRIPOS>BOND
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   2    5   19   1
   3    4   19   1
   4   19    6   1
   5   19   26   1
   6   20    7   1
   7   20    9   1
   8   20   26   1
   9   26    1   1
  10   26   25   1
  11   17    1   1
  12    3   18   1
  13    1   22   1
  14    1   21   1
  15   18   22   2
  16   18    2   1
  17   22   23   1
  18   12   23   1
  19   25   16   1
  20   25   21   1
  21   25   24   1
  22   14   24   1
```

23	23	24	1
24	23	13	1
25	10	21	1
26	21	11	1
27	24	15	1

Compound 10

@<TRIPOS>MOLECULE
compuesto_10.out
 26 25 0 0 0
SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM
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    1 C     -8.9510   0.4149 -11.4624 C.2    1 UNL1    -0.3134
    2 H     -4.4464  -1.6289  -4.2633 H      1 UNL1     0.1618
    3 H     -3.0511  -1.6234  -5.3524 H      1 UNL1     0.1618
    4 H     -4.6598  -1.9887  -5.9779 H      1 UNL1     0.1597
    5 H     -8.0760  -1.9405 -10.3402 H      1 UNL1     0.1565
    6 H     -6.9810  -2.0782  -8.9238 H      1 UNL1     0.1569
    7 H     -2.4908   0.8285  -4.6270 H      1 UNL1     0.1619
    8 H     -3.8827   0.8256  -3.5361 H      1 UNL1     0.1620
    9 H     -3.7357   2.0710  -4.7801 H      1 UNL1     0.1584
   10 H     -5.1772   1.6946  -6.6176 H      1 UNL1     0.1503
   11 H     -6.5634  -0.8701  -6.9527 H      1 UNL1     0.1407
   12 H     -5.1635  -0.8684  -8.0496 H      1 UNL1     0.1406
   13 H     -7.3206   1.3400  -7.9212 H      1 UNL1     0.1513
   14 H     -5.9212   1.3444  -9.0106 H      1 UNL1     0.1513
   15 H     -8.0274   1.8812 -10.2720 H      1 UNL1     0.1413
   16 H     -9.1435  -0.6187 -11.7133 H      1 UNL1     0.1517
   17 H     -9.4613   1.1117 -12.1135 H      1 UNL1     0.1473
   18 C     -4.1128  -1.3522  -5.2727 C.3    1 UNL1    -0.5009
   19 C     -7.4987  -1.4124  -9.5952 C.2    1 UNL1    -0.4076
   20 C     -3.5725   1.0065  -4.5753 C.3    1 UNL1    -0.5041
   21 C     -4.3145   0.1102  -5.5237 C.2    1 UNL1     0.1288
   22 C     -5.0825   0.6147  -6.5012 C.2    1 UNL1    -0.2763
   23 C     -5.8565  -0.2020  -7.4928 C.3    1 UNL1    -0.2210
   24 C     -6.6350   0.6724  -8.4871 C.3    1 UNL1    -0.3095
   25 C     -7.4405  -0.0779  -9.5222 C.2    1 UNL1     0.1003
   26 C     -8.1681   0.8106 -10.4568 C.2    1 UNL1    -0.1497
```
@<TRIPOS>BOND
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    5  26  25   1
    6   5  19   1
    7  19  25   2
    8  19   6   1
    9  25  24   1
   10  14  24   1
   11  24  13   1
   12  24  23   1
   13  12  23   1
   14  23  11   1
   15  23  22   1
   16  10  22   1
   17  22  21   2
   18   4  18   1
   19  21  18   1
   20  21  20   1
   21   3  18   1
   22  18   2   1
   23   9  20   1
   24   7  20   1
   25  20   8   1
```

Compound 11

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@<TRIPOS>MOLECULE
compuesto_11.out
 26 26 0 0 0
SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM
    1 C    -11.1593   -0.0043  -14.3008 C.3    1  UNL1    -0.2560
    2 H     -9.2875    4.0841  -12.8206 H      1  UNL1     0.1620
    3 H     -8.2822    2.8516  -13.6067 H      1  UNL1     0.1626
    4 H     -8.7395    2.6754  -11.8802 H      1  UNL1     0.1638
    5 H    -12.4037    2.3047  -13.7563 H      1  UNL1     0.1601
    6 H    -11.6011    3.9067  -13.3855 H      1  UNL1     0.1564
    7 H    -10.0298   -4.0939  -12.2815 H      1  UNL1     0.1589
    8 H     -9.5634   -3.9769  -13.9972 H      1  UNL1     0.1614
    9 H    -11.2959   -4.0882  -13.5292 H      1  UNL1     0.1618
   10 H     -9.1239    0.5426  -13.8626 H      1  UNL1     0.1362
   11 H     -9.2864    0.3886  -11.4166 H      1  UNL1     0.1333
   12 H    -11.0791    0.3516  -11.4560 H      1  UNL1     0.1454
   13 H     -9.8959   -1.9891  -11.1582 H      1  UNL1     0.1439
   14 H    -11.5853   -2.0151  -14.9971 H      1  UNL1     0.1418
   15 H     -9.8649   -1.5353  -15.1798 H      1  UNL1     0.1446
   16 H    -12.1671    0.0227  -13.8294 H      1  UNL1     0.1404
   17 H    -11.2331    0.5000  -15.2898 H      1  UNL1     0.1322
   18 C     -9.0978    2.9984  -12.8726 C.3    1  UNL1    -0.5086
   19 C    -11.4944    2.8355  -13.4870 C.2    1  UNL1    -0.4499
   20 C    -10.3242    2.2159  -13.2746 C.2    1  UNL1     0.1286
   21 C    -10.3140   -3.6556  -13.2491 C.3    1  UNL1    -0.5006
   22 C    -10.1378    0.7125  -13.3991 C.3    1  UNL1    -0.1130
   23 C    -10.1641    0.0450  -12.0085 C.3    1  UNL1    -0.2447
   24 C    -10.1367   -1.4567  -12.0872 C.2    1  UNL1    -0.2526
   25 C    -10.3943   -2.1526  -13.2054 C.2    1  UNL1     0.0873
   26 C    -10.7473   -1.4713  -14.5050 C.3    1  UNL1    -0.2952
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    4   26    1  1
    5   26   25  1
    6    1   16  1
    7    1   22  1
    8    8   21  1
    9   10   22  1
   10    5   19  1
   11    3   18  1
   12    9   21  1
   13   19    6  1
   14   19   20  2
   15   22   20  1
   16   22   23  1
   17   20   18  1
   18   21   25  1
   19   21    7  1
   20   25   24  2
   21   18    2  1
   22   18    4  1
   23   24   23  1
   24   24   13  1
   25   23   12  1
   26   23   11  1
```

Compound 12

```
@<TRIPOS>MOLECULE
compuesto_12.out
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SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM
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    1 C     -8.9637    0.0801   -0.8023 C.ar   1 UNL1      -0.1563
    2 C     -8.4561   -1.1909   -0.5307 C.ar   1 UNL1      -0.2060
    3 C     -9.1386   -2.0666    0.3253 C.ar   1 UNL1       0.0995
    4 C    -10.3511   -1.6502    0.8978 C.ar   1 UNL1      -0.2104
    5 C    -10.8574   -0.3805    0.6248 C.ar   1 UNL1      -0.1399
    6 C    -10.1710    0.4985   -0.2308 C.ar   1 UNL1      -0.0176
    7 C    -10.7202    1.8707   -0.5351 C.3    1 UNL1      -0.0043
    8 C    -12.0843    1.7660   -1.2352 C.3    1 UNL1      -0.4875
    9 C    -10.8027    2.7008    0.7536 C.3    1 UNL1      -0.4886
   10 C     -8.5799   -3.4213    0.6301 C.3    1 UNL1      -0.4980
   11 H     -8.4071    0.7478   -1.4530 H      1 UNL1       0.1439
   12 H     -7.5183   -1.5069   -0.9841 H      1 UNL1       0.1488
   13 H    -10.9051   -2.3187    1.5535 H      1 UNL1       0.1491
   14 H    -11.7945   -0.0678    1.0829 H      1 UNL1       0.1448
   15 H    -10.0251    2.4017   -1.2327 H      1 UNL1       0.1192
   16 H    -12.4586    2.7520   -1.5267 H      1 UNL1       0.1489
   17 H    -12.0088    1.1515   -2.1422 H      1 UNL1       0.1539
   18 H    -12.8400    1.3012   -0.5937 H      1 UNL1       0.1527
   19 H    -11.1255    3.7245    0.5498 H      1 UNL1       0.1486
   20 H     -9.8208    2.7486    1.2482 H      1 UNL1       0.1543
   21 H    -11.5041    2.2758    1.4774 H      1 UNL1       0.1526
   22 H     -7.4874   -3.4451    0.5875 H      1 UNL1       0.1619
   23 H     -8.8711   -3.7746    1.6343 H      1 UNL1       0.1629
   24 H     -8.9619   -4.1573   -0.1033 H      1 UNL1       0.1673
```
@<TRIPOS>BOND
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    5    8    7   1
    6   15    7   1
    7   12    2   1
    8    1    2  ar
    9    1    6  ar
   10    7    6   1
   11    7    9   1
   12    2    3  ar
   13    6    5  ar
   14   24   10   1
   15    3   10   1
   16    3    4  ar
   17   19    9   1
   18   22   10   1
   19    5    4  ar
   20    5   14   1
   21   10   23   1
   22    9   20   1
   23    9   21   1
   24    4   13   1
```

Compound 13

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compuesto_13.out
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SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM
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    1 C     -7.6969   -0.8923  -11.3083 C.3    1 UNL1      -0.3729
    2 H     -7.8926    2.6883   -7.5181 H      1 UNL1       0.1628
    3 H     -6.7495    1.4234   -7.1334 H      1 UNL1       0.1524
    4 H     -8.4063    0.8486   -7.2900 H      1 UNL1       0.1978
```

5 H	-7.7744	3.3451	-10.0070	H	1	UNL1	0.1613
6 H	-9.3155	2.5102	-9.7040	H	1	UNL1	0.1698
7 H	-8.3912	1.9402	-11.0720	H	1	UNL1	0.1691
8 H	-5.5657	1.5650	-9.9285	H	1	UNL1	0.1308
9 H	-5.4739	-0.1027	-8.0594	H	1	UNL1	0.1315
10 H	-4.8000	-0.8674	-9.5204	H	1	UNL1	0.1261
11 H	-5.6658	0.0530	-11.8252	H	1	UNL1	0.1292
12 H	-7.1104	0.9529	-11.9563	H	1	UNL1	0.1279
13 H	-6.2512	-2.3648	-9.8344	H	1	UNL1	0.1409
14 H	-6.9321	-2.2360	-8.2443	H	1	UNL1	0.1492
15 H	-8.5695	-0.4549	-11.8393	H	1	UNL1	0.1490
16 H	-7.4488	-1.8657	-11.7967	H	1	UNL1	0.1469
17 C	-9.3190	-1.9644	-9.5738	C.3	1	UNL1	-0.5677
18 C	-7.6605	1.6005	-7.7066	C.3	1	UNL1	-0.5622
19 C	-8.2849	2.3442	-10.0439	C.3	1	UNL1	-0.5689
20 C	-7.6124	1.2410	-9.2033	C.3	1	UNL1	0.4385
21 O	-8.5108	0.0933	-9.2337	O.3	1	UNL1	-0.5757
22 C	-6.2952	0.7328	-9.8705	C.3	1	UNL1	-0.1715
23 C	-5.7341	-0.4664	-9.0714	C.3	1	UNL1	-0.2302
24 C	-6.6198	0.2196	-11.3101	C.3	1	UNL1	-0.2473
25 C	-6.7380	-1.6423	-9.1576	C.3	1	UNL1	-0.3673
26 C	-8.0430	-1.1609	-9.8320	C.3	1	UNL1	0.4480
27 H	-9.7414	-1.3944	-8.6917	H	1	UNL1	0.2025
28 H	-10.0419	-1.8073	-10.3814	H	1	UNL1	0.1639
29 H	-9.2520	-3.0682	-9.4309	H	1	UNL1	0.1660

@<TRIPOS>BOND
```
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 3   11  24   1
 4   16   1   1
 5   24   1   1
 6   24  22   1
 7    1  26   1
 8    7  19   1
 9   28  17   1
10   19   5   1
11   19   6   1
12   19  20   1
13    8  22   1
14   22  20   1
15   22  23   1
16   13  25   1
17   26  17   1
18   26  21   1
19   26  25   1
20   17  29   1
21   17  27   1
22   10  23   1
23   21  20   1
24   20  18   1
25   25  23   1
26   25  14   1
27   23   9   1
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30   18   3   1
```

Compound 14

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compuesto_14.out
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SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM
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  1 C    -7.2468   0.0097  -9.4289 C.3   1 UNL1    0.4030
```

2 H	-7.4671	2.1241	-8.8997 H	1 UNL1	0.1562
3 H	-8.0350	0.1206	-11.2908 H	1 UNL1	0.3106
4 H	-7.7147	-1.5968	-8.1067 H	1 UNL1	0.1760
5 H	-7.4237	-2.1368	-9.7639 H	1 UNL1	0.1729
6 H	-8.9792	-1.3737	-9.4130 H	1 UNL1	0.1648
7 H	-2.2371	0.2522	-5.1820 H	1 UNL1	0.1660
8 H	-3.3942	1.1875	-4.2392 H	1 UNL1	0.1581
9 H	-3.0001	1.7189	-5.8872 H	1 UNL1	0.1652
10 H	-3.2964	-0.1791	-7.6869 H	1 UNL1	0.1513
11 H	-6.1600	-1.2518	-7.3097 H	1 UNL1	0.1316
12 H	-4.9654	-1.9005	-8.4323 H	1 UNL1	0.1328
13 H	-5.4193	1.0498	-8.7755 H	1 UNL1	0.1596
14 H	-5.2143	-0.1971	-10.0119 H	1 UNL1	0.1698
15 C	-5.5347	-0.0631	-4.9916 C.3	1 UNL1	-0.4999
16 C	-9.1265	1.0844	-8.1017 C.2	1 UNL1	-0.3176
17 C	-7.9847	1.1650	-8.7796 C.2	1 UNL1	-0.2012
18 O	-7.1840	0.2806	-10.8536 O.3	1 UNL1	-0.5947
19 C	-7.9007	-1.3479	-9.1719 C.3	1 UNL1	-0.5756
20 C	-3.1751	0.8361	-5.2527 C.3	1 UNL1	-0.5132
21 C	-4.3272	0.0862	-5.8655 C.2	1 UNL1	0.1443
22 C	-4.2242	-0.3344	-7.1354 C.2	1 UNL1	-0.2911
23 C	-5.3105	-0.9555	-7.9576 C.3	1 UNL1	-0.2125
24 C	-5.7440	0.0270	-9.0619 C.3	1 UNL1	-0.3420
25 H	-9.5404	1.9339	-7.5774 H	1 UNL1	0.1478
26 H	-9.7284	0.1889	-8.0024 H	1 UNL1	0.1492
27 H	-5.2459	-0.6239	-4.0819 H	1 UNL1	0.1634
28 H	-5.9079	0.9179	-4.6586 H	1 UNL1	0.1621
29 H	-6.3865	-0.5561	-5.5008 H	1 UNL1	0.1628

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 8   6  19  1
 9  19   4  1
10  24  13  1
11  24  23  1
12   2  17  1
13  17  16  2
14  12  23  1
15  16  26  1
16  16  25  1
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18  23  22  1
19  10  22  1
20  22  21  2
21   9  20  1
22  21  20  1
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Compound 15

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MULLIKEN_CHARGES

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1 C	-9.3721	1.0777	-12.7652	C.3	1 UNL1	-0.4978
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3 H	-8.9770	-2.0372	-11.1977	H	1 UNL1	0.1515
4 H	-8.0420	-1.4026	-12.5777	H	1 UNL1	0.1550
5 H	-9.8162	-1.6259	-12.7178	H	1 UNL1	0.1539
6 H	-6.0720	1.4942	-6.0649	H	1 UNL1	0.1847
7 H	-4.8924	1.1926	-7.3903	H	1 UNL1	0.1878
8 H	-8.8652	-0.1557	-8.7927	H	1 UNL1	0.1317
9 H	-7.5760	-1.2213	-9.5615	H	1 UNL1	0.1344
10 H	-8.2424	1.7021	-10.3935	H	1 UNL1	0.1557
11 H	-7.0917	0.5786	-11.2210	H	1 UNL1	0.1554
12 H	-10.1447	0.1418	-10.9400	H	1 UNL1	0.1104
13 H	-10.2463	0.7481	-13.3994	H	1 UNL1	0.1539
14 H	-8.4785	1.0868	-13.3812	H	1 UNL1	0.1538
15 H	-9.5887	2.1070	-12.4323	H	1 UNL1	0.1502
16 C	-3.8662	-1.2286	-6.4998	C.3	1 UNL1	-0.5051
17 C	-3.6645	0.7772	-4.9372	C.3	1 UNL1	-0.5062
18 C	-4.6436	-0.1545	-5.7005	C.3	1 UNL1	0.0643
19 O	-7.1870	-1.0818	-6.9124	O.2	1 UNL1	-0.5243
20 C	-8.9843	-1.3266	-12.0473	C.3	1 UNL1	-0.5007
21 C	-5.5583	0.7022	-6.6587	C.3	1 UNL1	-0.4445
22 C	-6.6155	-0.1154	-7.3469	C.2	1 UNL1	0.6496
23 O	-6.8965	0.4604	-8.5603	O.3	1 UNL1	-0.4625
24 C	-7.9047	-0.1735	-9.3605	C.3	1 UNL1	-0.0050
25 C	-8.0432	0.6337	-10.6629	C.3	1 UNL1	-0.3398
26 C	-9.2187	0.1180	-11.5584	C.3	1 UNL1	0.0302
27 H	-4.2202	1.5385	-4.3462	H	1 UNL1	0.1529
28 H	-3.0521	0.1880	-4.2525	H	1 UNL1	0.1567
29 H	-3.0028	1.3031	-5.6511	H	1 UNL1	0.1558
30 H	-4.5618	-1.9267	-7.0151	H	1 UNL1	0.1632
31 H	-3.2229	-0.7665	-7.2456	H	1 UNL1	0.1520
32 H	-3.2318	-1.8332	-5.7959	H	1 UNL1	0.1576

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 7   20  26   1
 8   20   3   1
 9   26  12   1
10   26  25   1
11   11  25   1
12   25  10   1
13   25  24   1
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18    7  21   1
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20   22  21   1
21   31  16   1
22   30  16   1
23   21   6   1
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25   16  32   1
26   16  18   1
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Compound 16

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SMALL
MULLIKEN_CHARGES

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    2 C     -10.6733   1.3528 -14.6932 C.3    1 UNL1    -0.5050
    3 C      -8.7035   1.2580 -13.1846 C.3    1 UNL1    -0.5196
    4 C      -9.3012  -1.5844 -14.5444 C.3    1 UNL1    -0.4740
    5 O      -9.0396  -2.1562 -11.6580 O.2    1 UNL1    -0.4839
    6 H     -12.0267  -1.2531 -14.5411 H      1 UNL1     0.1431
    7 H     -11.8327  -2.2467 -13.0708 H      1 UNL1     0.1399
    8 H     -10.9773  -0.5793 -10.3768 H      1 UNL1     0.1774
    9 H      -9.5202   0.4333 -10.6174 H      1 UNL1     0.1772
   10 H     -12.8527  -0.5135 -11.7846 H      1 UNL1     0.1371
   11 H     -12.9748   0.4983 -13.2633 H      1 UNL1     0.1363
   12 H     -11.3066   1.7240 -11.8568 H      1 UNL1     0.1271
   13 H     -10.0008   1.2304 -15.5650 H      1 UNL1     0.1573
   14 H     -11.6592   0.9769 -15.0097 H      1 UNL1     0.1559
   15 H     -10.8127   2.4356 -14.4776 H      1 UNL1     0.1544
   16 H      -8.1271   0.7390 -12.3905 H      1 UNL1     0.1582
   17 H      -8.0918   1.2063 -14.0977 H      1 UNL1     0.1595
   18 H      -8.8055   2.3246 -12.9001 H      1 UNL1     0.1574
   19 H      -8.2271  -1.3434 -14.4307 H      1 UNL1     0.1609
   20 H      -9.3962  -2.6877 -14.4687 H      1 UNL1     0.1639
   21 H      -9.6223  -1.2759 -15.5579 H      1 UNL1     0.1546
   22 C     -10.1001   0.6615 -13.4462 C.3    1 UNL1     0.1604
   23 C     -11.0581   0.7128 -12.1932 C.3    1 UNL1    -0.0927
   24 C     -12.2857  -0.1200 -12.6512 C.3    1 UNL1    -0.2840
   25 C     -10.3119  -0.1398 -11.1380 C.3    1 UNL1    -0.4589
   26 C      -9.7105  -1.2273 -12.0207 C.2    1 UNL1     0.5282
   27 C     -10.1272  -0.9046 -13.4750 C.3    1 UNL1    -0.0526
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Compound 17

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      3 C      -6.6057   -2.1067   -9.2613 C.3    1 UNL1       0.0276
      4 C      -6.6888   -1.5568   -7.8243 C.3    1 UNL1      -0.3177
      5 C      -6.4930   -0.0289   -7.7891 C.3    1 UNL1      -0.2381
      6 C      -6.9521    0.6820   -9.0827 C.3    1 UNL1      -0.2801
      7 C      -7.2078    2.2009   -8.8969 C.3    1 UNL1       0.0348
      8 C      -7.4387    2.9021  -10.2539 C.3    1 UNL1      -0.5039
      9 C      -6.0370    2.9077   -8.1806 C.3    1 UNL1      -0.5001
     10 C      -6.6085   -3.6429   -9.2822 C.3    1 UNL1      -0.5048
     11 O      -9.2319    0.3379   -9.8027 O.2    1 UNL1      -0.5003
     12 H      -8.6973   -2.1604   -9.8953 H      1 UNL1       0.1857
     13 H      -7.5602   -1.5571  -11.1619 H      1 UNL1       0.1755
     14 H      -5.6456   -1.7573   -9.7115 H      1 UNL1       0.1137
     15 H      -7.6871   -1.8241   -7.4054 H      1 UNL1       0.1456
     16 H      -5.9235   -2.0417   -7.1758 H      1 UNL1       0.1405
     17 H      -7.0549    0.3731   -6.9106 H      1 UNL1       0.1401
     18 H      -5.4164    0.2023   -7.6232 H      1 UNL1       0.1358
     19 H      -6.1363    0.5873   -9.8420 H      1 UNL1       0.1575
     20 H      -8.1214    2.3330   -8.2686 H      1 UNL1       0.1255
     21 H      -8.2976    2.4617  -10.8172 H      1 UNL1       0.1661
     22 H      -7.6664    3.9807  -10.1133 H      1 UNL1       0.1526
     23 H      -6.5394    2.8303  -10.9046 H      1 UNL1       0.1459
     24 H      -5.9017    2.5398   -7.1395 H      1 UNL1       0.1475
     25 H      -5.0825    2.7482   -8.7257 H      1 UNL1       0.1501
     26 H      -6.2158    4.0074   -8.1150 H      1 UNL1       0.1540
     27 H      -6.5640   -4.0284  -10.3274 H      1 UNL1       0.1548
     28 H      -5.7264   -4.0495   -8.7421 H      1 UNL1       0.1537
     29 H      -7.5231   -4.0475   -8.8020 H      1 UNL1       0.1566
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Compound 18

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MULLIKEN_CHARGES

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   3 H       -8.2725  -4.0529  -9.7651 H      1 UNL1     0.1563
   4 C       -8.8742  -0.1048 -10.6267 C.2    1 UNL1     0.5634
   5 C       -8.5422  -1.5338 -11.0333 C.3    1 UNL1    -0.4821
   6 C       -7.3597  -2.1063 -10.2261 C.3    1 UNL1     0.0276
   7 C       -7.4443  -1.5581  -8.7877 C.3    1 UNL1    -0.3177
   8 C       -7.2465  -0.0293  -8.7536 C.3    1 UNL1    -0.2381
   9 C       -7.7043   0.6818 -10.0483 C.3    1 UNL1    -0.2797
  10 C       -7.9632   2.2014  -9.8629 C.3    1 UNL1     0.0355
  11 C       -8.1919   2.8987 -11.2203 C.3    1 UNL1    -0.5043
  12 C       -6.7917   2.9068  -9.1457 C.3    1 UNL1    -0.5007
  13 C       -7.3620  -3.6433 -10.2491 C.3    1 UNL1    -0.5049
  14 O       -9.9899   0.3369 -10.7685 O.2    1 UNL1    -0.5016
  15 H       -9.4538  -2.1591 -10.8667 H      1 UNL1     0.1857
  16 H       -8.3117  -1.5598 -12.1248 H      1 UNL1     0.1755
  17 H       -6.3959  -1.7569 -10.6763 H      1 UNL1     0.1140
  18 H       -8.4429  -1.8269  -8.3727 H      1 UNL1     0.1456
  19 H       -6.6783  -2.0417  -8.1352 H      1 UNL1     0.1406
  20 H       -7.8125   0.3734  -7.8817 H      1 UNL1     0.1398
  21 H       -6.1648   0.2005  -8.5848 H      1 UNL1     0.1364
  22 H       -6.8894   0.5915 -10.8069 H      1 UNL1     0.1577
  23 H       -8.8761   2.3284  -9.2354 H      1 UNL1     0.1254
  24 H       -9.0525   2.4679 -11.7843 H      1 UNL1     0.1665
  25 H       -8.4146   3.9812 -11.0790 H      1 UNL1     0.1528
  26 H       -7.2914   2.8301 -11.8647 H      1 UNL1     0.1460
  27 H       -6.6667   2.5442  -8.1055 H      1 UNL1     0.1477
  28 H       -5.8374   2.7491  -9.6895 H      1 UNL1     0.1505
  29 H       -6.9642   4.0033  -9.0787 H      1 UNL1     0.1535
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Compound 19

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SMALL
MULLIKEN_CHARGES

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      3 O      6.3912  -2.6868   9.9712 O.3   1 UNL1       -0.5619
      4 C      5.1452  -1.1316  12.4338 C.3   1 UNL1       -0.5085
      5 C      6.1899   1.8937  11.9540 C.3   1 UNL1       -0.5069
      6 C      4.4634   1.2279  10.3171 C.3   1 UNL1       -0.5128
      7 H      4.7021  -1.5289   9.7734 H     1 UNL1        0.0965
      8 H      7.7668  -0.3667  12.6408 H     1 UNL1        0.1284
      9 H      7.9383  -1.7583  11.5448 H     1 UNL1        0.1545
     10 H      7.2740  -0.9677   8.3732 H     1 UNL1        0.1564
     11 H      5.7225  -0.1527   8.1507 H     1 UNL1        0.1367
     12 H      8.9000  -0.3360   9.9122 H     1 UNL1        0.1348
     13 H      8.7427   1.0296  11.0023 H     1 UNL1        0.1253
     14 H      7.1447   1.6171   9.1886 H     1 UNL1        0.1191
     15 H      6.0819  -3.1822   9.1875 H     1 UNL1        0.3046
     16 H      4.0853  -0.9662  12.2328 H     1 UNL1        0.1526
     17 H      5.3282  -2.1913  12.6454 H     1 UNL1        0.1674
     18 H      5.3243  -0.5690  13.3451 H     1 UNL1        0.1541
     19 H      6.2557   2.9079  11.5526 H     1 UNL1        0.1515
     20 H      5.4327   1.8888  12.7430 H     1 UNL1        0.1521
     21 H      7.1507   1.6625  12.4212 H     1 UNL1        0.1587
     22 H      3.7298   1.2532  11.1366 H     1 UNL1        0.1543
     23 H      4.5240   2.2347   9.8840 H     1 UNL1        0.1541
     24 H      4.0815   0.5423   9.5390 H     1 UNL1        0.1517
     25 C      6.9614   0.7139   9.7626 C.3   1 UNL1       -0.0959
     26 C      8.1936   0.2002  10.5559 C.3   1 UNL1       -0.2748
     27 C      6.4541  -0.4692   8.9029 C.3   1 UNL1       -0.3722
     28 C      5.7862  -1.3877   9.9527 C.3   1 UNL1        0.1460
     29 C      6.0322  -0.6533  11.3090 C.3   1 UNL1        0.0845
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 23    9    1   1
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 25    1    8   1
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Compound 20

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SMALL
MULLIKEN_CHARGES

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      2 C      5.3891  -2.2037   9.7823 C.3    1 UNL1       0.0171
      3 C      6.3248  -2.8841  10.8058 C.3    1 UNL1      -0.5009
      4 C      5.5410  -2.9695   8.4530 C.3    1 UNL1      -0.4928
      5 H      4.8483   1.8105  11.3364 H      1 UNL1       0.1363
      6 H      6.5726   1.9799  11.7145 H      1 UNL1       0.1345
      7 H      5.3695  -0.4126  11.7898 H      1 UNL1       0.1338
      8 H      7.0589  -0.2569  11.2486 H      1 UNL1       0.1348
      9 H      6.5637  -0.5936   8.9588 H      1 UNL1       0.1434
     10 H      3.6935   0.2144   9.7524 H      1 UNL1       0.0980
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     15 H      5.1485   4.0549   9.9709 H      1 UNL1       0.1536
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     17 H      3.3091   0.1215   7.4773 H      1 UNL1       0.3087
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     19 H      6.1662  -3.9766  10.8421 H      1 UNL1       0.1490
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    4 H      5.4289  -0.0519  12.5293 H      1 UNL1       0.1475
    5 H      7.1288  -0.4099  12.9370 H      1 UNL1       0.1262
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   11 H      5.7898   4.2013  10.0433 H      1 UNL1       0.1488
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   14 H      5.1782  -2.2949  11.3463 H      1 UNL1       0.1294
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   16 H      6.8940  -4.0506  12.0374 H      1 UNL1       0.1496
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   19 H      7.3061  -2.8972   9.1745 H      1 UNL1       0.1466
   20 H      6.1077  -4.0818   9.7612 H      1 UNL1       0.1496
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   22 O      4.4305  -0.1443   9.9729 O.3    1 UNL1      -0.5661
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   24 C      7.1285  -2.9665  11.9991 C.3    1 UNL1      -0.4984
   25 C      6.2327  -2.2440  10.9783 C.3    1 UNL1       0.0092
   26 C      6.4121   3.6937  10.8029 C.3    1 UNL1      -0.5087
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      4 H      6.4118   -2.3069    8.9675 H       1 UNL1       0.1609
      5 H      5.3898   -2.7568   13.0019 H       1 UNL1       0.1665
      6 H      7.1568   -2.6350   13.0160 H       1 UNL1       0.1683
      7 H      6.3459   -3.9669   12.2316 H       1 UNL1       0.1624
      8 H      4.9656    2.1156    9.5081 H       1 UNL1       0.1403
      9 H      4.7361   -0.3211    9.5889 H       1 UNL1       0.1546
     10 H      6.4386   -0.0588    9.0847 H       1 UNL1       0.1625
     11 H      5.2895   -0.4683   11.9482 H       1 UNL1       0.1391
     12 H      7.6664   -0.4272   12.7442 H       1 UNL1       0.1804
     13 H      8.2337   -0.1436   11.0474 H       1 UNL1       0.1821
     14 C      6.2178    3.7200   11.2284 C.3     1 UNL1      -0.4358
     15 O      7.9317    2.1277   12.7209 O.2     1 UNL1      -0.4907
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     17 C      6.2935   -2.9056   12.3955 C.3     1 UNL1      -0.5122
     18 C      6.2919   -2.1580   11.0930 C.2     1 UNL1       0.1247
     19 C      6.3435    2.2386   11.0631 C.2     1 UNL1      -0.1634
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     21 C      5.7137    0.0843    9.9115 C.3     1 UNL1      -0.3068
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Compound 23

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   4 H      6.4171  -3.8959  11.1945 H      1 UNL1       0.1502
   5 H      6.8055  -2.4601  12.1054 H      1 UNL1       0.1464
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  27 C      5.9470  -0.5929  10.0053 C.3    1 UNL1      -0.1620
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  30 H      2.9552  -1.3779   6.2495 H      1 UNL1       0.1964
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  32 H      5.9859  -2.7874   8.2890 H      1 UNL1       0.1500
  33 H      5.1402  -4.0013   9.3114 H      1 UNL1       0.1438
  34 C      5.5784   2.3620  10.6270 C.3    1 UNL1       0.0016
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Compound 24

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   12 H      6.2935   4.0757  11.3586 H     1 UNL1     0.1516
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   17 H      8.2061  -2.6531  10.3572 H     1 UNL1     0.1463
   18 H      7.0974  -4.0203  10.5143 H     1 UNL1     0.1456
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   25 H      7.3825  -0.4339   9.7910 H     1 UNL1     0.1259
   26 H      5.2569   1.8954  13.3473 H     1 UNL1     0.1440
   27 H      6.6707   2.9710  13.3587 H     1 UNL1     0.1461
   28 H      8.7661  -0.0160  11.7994 H     1 UNL1     0.1562
   29 H      6.7980   1.2557  15.3736 H     1 UNL1     0.1478
   30 C      7.1498   3.5973  10.8725 C.3   1 UNL1    -0.4917
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33 C	7.2204	-2.9539	10.7258	C.3	1	UNL1	-0.4947
34 C	6.0972	-2.1233	10.0853	C.3	1	UNL1	-0.0024
35 H	5.7566	-0.6722	12.3977	H	1	UNL1	0.1548
36 C	9.9411	2.0957	10.6668	C.3	1	UNL1	-0.0309
37 C	5.6752	1.8196	9.8175	C.3	1	UNL1	-0.2822
38 C	5.3644	0.3207	9.6069	C.3	1	UNL1	-0.2742
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4 H	5.6828	-2.5405	-15.3207	H	1	UNL1	0.1478
5 H	3.9855	-2.3354	-15.7882	H	1	UNL1	0.1569
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 9 H      4.5129   2.0599 -14.8507 H    1 UNL1    0.1366
10 H      6.1423   1.3660 -12.3136 H    1 UNL1    0.1372
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12 H      1.8544   0.2108 -10.8462 H    1 UNL1    0.1424
13 H      3.2462   2.3837 -12.6331 H    1 UNL1    0.1257
14 H      2.8224  -0.1747 -14.4354 H    1 UNL1    0.1308
15 H      1.2915   0.0336 -12.5190 H    1 UNL1    0.1394
16 H      2.2323  -2.4177 -11.3449 H    1 UNL1    0.1501
17 H      3.9373  -2.6436 -13.4697 H    1 UNL1    0.1543
18 C      4.0858   2.1142 -10.6620 C.3  1 UNL1   -0.4854
19 C      5.0119  -2.0197 -16.0128 C.3  1 UNL1   -0.4968
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21 C      5.1616  -0.4966 -15.9042 C.3  1 UNL1   -0.0034
22 C      5.2565  -1.3168 -10.8107 C.3  1 UNL1   -0.4585
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26 C      5.3566   1.9328 -12.8478 C.3  1 UNL1   -0.2790
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 3    2  20  1
 4   20   1  1
 5   20  21  1
 6   35  21  1
 7   19  21  1
 8   19   5  1
 9   19   4  1
10   21  24  1
11    9  25  1
12    8  25  1
13   14  28  1
14   24  25  1
15   24   7  1
16   24  28  1
17   25  26  1
18   28   6  1
19   28  29  1
20   17   6  1
21    6  31  1
22    6  23  1
23   26  11  1
24   26  10  1
25   26  27  1
26   13  27  1
27   15  30  1
28   29  27  1
29   29  30  1
30   29  23  1
31   27  18  1
32   30  31  1
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33	30	12	1
34	31	23	1
35	31	16	1
36	23	22	1
37	32	22	1
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42	18	38	1

Compound 26

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compuesto_26.out
 33 35 0 0 0
SMALL
MULLIKEN_CHARGES

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     1 C      4.8432   0.8433 -16.5720 C.2    1 UNL1      -0.2534
     2 C      3.7283  -0.1352 -16.2996 C.3    1 UNL1      -0.2527
     3 C      3.7060  -0.5343 -14.8089 C.3    1 UNL1      -0.1393
     4 C      5.1574  -0.8901 -14.3339 C.3    1 UNL1      -0.1270
     5 C      5.3597   0.6602 -14.1828 C.3    1 UNL1      -0.2046
     6 C      5.6272   1.2430 -15.5519 C.2    1 UNL1       0.0845
     7 C      5.2112  -1.6027 -12.9680 C.3    1 UNL1      -0.0374
     8 C      4.0018  -1.1898 -12.0992 C.3    1 UNL1      -0.2794
     9 C      3.6206   0.2778 -12.3579 C.3    1 UNL1      -0.3136
    10 C      3.8247   0.6955 -13.8368 C.3    1 UNL1       0.1579
    11 C      6.7442   2.2225 -15.6917 C.3    1 UNL1      -0.4979
    12 C      3.0686   1.9656 -14.1575 C.3    1 UNL1      -0.5204
    13 C      5.2752  -3.1233 -13.1369 C.3    1 UNL1      -0.4960
    14 H      2.9208  -1.2579 -14.5761 H      1 UNL1       0.1273
    15 H      6.0466   0.9924 -13.4003 H      1 UNL1       0.1361
    16 H      5.8087  -1.3593 -15.0795 H      1 UNL1       0.1331
    17 H      4.9714   1.2064 -17.5871 H      1 UNL1       0.1430
    18 H      2.7538   0.3076 -16.5874 H      1 UNL1       0.1378
    19 H      3.8658  -1.0459 -16.9175 H      1 UNL1       0.1366
    20 H      6.1468  -1.2706 -12.4511 H      1 UNL1       0.1172
    21 H      3.1343  -1.8340 -12.3467 H      1 UNL1       0.1345
    22 H      4.2091  -1.3596 -11.0247 H      1 UNL1       0.1277
    23 H      2.5650   0.4324 -12.0679 H      1 UNL1       0.1357
    24 H      4.2314   0.9448 -11.7173 H      1 UNL1       0.1373
    25 H      6.5749   3.1025 -15.0536 H      1 UNL1       0.1628
    26 H      7.7025   1.7677 -15.4010 H      1 UNL1       0.1634
    27 H      6.8358   2.5921 -16.7344 H      1 UNL1       0.1589
    28 H      1.9863   1.8170 -14.0662 H      1 UNL1       0.1530
    29 H      3.3655   2.7736 -13.4736 H      1 UNL1       0.1533
    30 H      3.2603   2.3310 -15.1788 H      1 UNL1       0.1696
    31 H      5.2918  -3.6313 -12.1616 H      1 UNL1       0.1485
    32 H      4.4024  -3.4974 -13.6982 H      1 UNL1       0.1535
    33 H      6.1776  -3.4214 -13.6893 H      1 UNL1       0.1500
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    6    1    6   2
    7    2    3   1
    8   11    6   1
    9   11   26   1
   10   11   25   1
   11    6    5   1
   12   30   12   1
   13   16    4   1
```

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15	3	4	1
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17	4	5	1
18	4	7	1
19	5	10	1
20	5	15	1
21	12	28	1
22	12	10	1
23	12	29	1
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26	33	13	1
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28	13	31	1
29	7	20	1
30	7	8	1
31	9	8	1
32	9	23	1
33	9	24	1
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35	8	22	1

Compound 27

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@<TRIPOS>MOLECULE
compuesto_27.out
 39 41 0 0 0
SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM
      1 C     2.2567  -0.0098   -9.9242 C.3    1 UNL1    -0.2972
      2 C     3.7951  -0.0607  -10.1895 C.3    1 UNL1     0.1190
      3 C     3.9897  -0.8787  -11.4462 C.2    1 UNL1    -0.0720
      4 H     3.9940   3.4228   -9.6290 H      1 UNL1     0.1489
      5 H     5.7580   0.9299  -11.9331 H      1 UNL1     0.1643
      6 H     6.2850   1.5388  -10.3741 H      1 UNL1     0.1502
      7 H     5.6187   2.6525  -11.5770 H      1 UNL1     0.1487
      8 H     2.2961   0.9630  -13.5120 H      1 UNL1     0.1421
      9 H     3.9514   1.5875  -13.5160 H      1 UNL1     0.1398
     10 H     1.0129   0.6835  -11.5946 H      1 UNL1     0.1324
     11 H     1.1752   1.8657  -10.2913 H      1 UNL1     0.1237
     12 H     2.0463   0.2186   -8.8679 H      1 UNL1     0.1294
     13 H     1.7852  -0.9811  -10.1338 H      1 UNL1     0.1362
     14 H     2.8147   2.7950  -11.7446 H      1 UNL1     0.1167
     15 C     3.1114  -1.4662  -14.9220 C.3    1 UNL1    -0.4870
     16 C     4.4080  -2.3246  -11.4960 C.3    1 UNL1    -0.2619
     17 C     4.2982  -2.7058  -12.9949 C.3    1 UNL1    -0.2851
     18 C     4.1060  -1.3657  -13.7696 C.3    1 UNL1    -0.0359
     19 C     4.5879  -0.5891   -9.0003 C.3    1 UNL1    -0.5055
     20 C     3.9937   2.3715   -9.3292 C.3    1 UNL1    -0.5165
     21 C     5.5184   1.6521  -11.1463 C.3    1 UNL1    -0.5157
     22 C     3.2288   1.0036  -12.9152 C.3    1 UNL1    -0.2853
     23 C     3.7421  -0.3792  -12.6763 C.2    1 UNL1    -0.0438
     24 C     4.1228   1.4458  -10.5521 C.3    1 UNL1     0.1603
     25 C     2.9584   1.7151  -11.5666 C.3    1 UNL1    -0.1066
     26 C     1.7211   1.0966  -10.8604 C.3    1 UNL1    -0.2710
     27 H     3.0734   2.1961   -8.7647 H      1 UNL1     0.1549
     28 H     4.8294   2.2282   -8.6367 H      1 UNL1     0.1508
     29 H     4.5146   0.0796   -8.1355 H      1 UNL1     0.1539
     30 H     4.2290  -1.5720   -8.6820 H      1 UNL1     0.1506
     31 H     5.6512  -0.6822   -9.2455 H      1 UNL1     0.1555
     32 H     5.0940  -1.0482  -14.1900 H      1 UNL1     0.1200
     33 H     3.4399  -3.3766  -13.1584 H      1 UNL1     0.1350
     34 H     5.1856  -3.2528  -13.3418 H      1 UNL1     0.1272
     35 H     5.4329  -2.4696  -11.1150 H      1 UNL1     0.1368
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36 H	3.7446	-2.9492	-10.8740 H	1 UNL1	0.1363
37 H	2.8181	-0.4767	-15.2922 H	1 UNL1	0.1505
38 H	3.5492	-2.0093	-15.7675 H	1 UNL1	0.1463
39 H	2.1931	-1.9871	-14.6292 H	1 UNL1	0.1542

@<TRIPOS>BOND
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 7   18  23   1
 8    9  22   1
 9    8  22   1
10   34  17   1
11   33  17   1
12   17  16   1
13   22  23   1
14   22  25   1
15   23   3   2
16    5  21   1
17   14  25   1
18   10  26   1
19    7  21   1
20   25  26   1
21   25  24   1
22   16   3   1
23   16  35   1
24   16  36   1
25    3   2   1
26   21  24   1
27   21   6   1
28   26  11   1
29   26   1   1
30   24   2   1
31   24  20   1
32    2   1   1
33    2  19   1
34   13   1   1
35    1  12   1
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41   19  29   1
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Compound 28

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compuesto_28.out
 39 41 0 0 0
SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM

1 C	3.0361	-0.0293	-10.7759 C.3	1 UNL1	-0.1418
2 H	5.4735	0.5083	-12.7711 H	1 UNL1	0.1374
3 H	3.8354	2.7116	-9.7469 H	1 UNL1	0.1482
4 H	5.4220	2.2914	-10.4105 H	1 UNL1	0.1448
5 H	5.1128	-0.0199	-10.0750 H	1 UNL1	0.1413
6 H	3.9450	0.5079	-8.8561 H	1 UNL1	0.1275
7 C	4.3488	-0.9404	-15.7417 C.3	1 UNL1	-0.4929
8 C	5.1187	1.4085	-15.2497 C.3	1 UNL1	-0.4957
9 C	3.9170	3.0983	-12.6754 C.2	1 UNL1	-0.4742
10 H	2.1146	-0.1300	-10.1847 H	1 UNL1	0.1262
11 H	1.8847	1.1599	-12.3070 H	1 UNL1	0.1386

12 H	2.7897	-0.4993	-13.7835 H	1	UNL1	0.1319
13 C	2.1390	-2.2119	-11.7731 C.3	1	UNL1	-0.5184
14 C	5.2332	-0.0666	-14.8447 C.3	1	UNL1	-0.0051
15 C	4.6571	-1.9989	-11.5726 C.3	1	UNL1	-0.3099
16 C	5.4398	-1.6711	-12.8556 C.3	1	UNL1	-0.2725
17 C	4.9324	-0.2873	-13.3435 C.3	1	UNL1	-0.1070
18 C	3.3205	-1.2576	-11.7031 C.3	1	UNL1	0.1291
19 C	3.4481	-0.2744	-12.9334 C.3	1	UNL1	-0.1363
20 C	2.9194	0.8839	-12.0437 C.3	1	UNL1	-0.1784
21 C	3.7665	2.1003	-11.8079 C.2	1	UNL1	0.1459
22 C	4.3601	2.0075	-10.4172 C.3	1	UNL1	-0.3063
23 C	4.1754	0.5540	-9.9304 C.3	1	UNL1	-0.2607
24 H	5.2375	-2.4492	-13.6150 H	1	UNL1	0.1327
25 H	6.5244	-1.6691	-12.6853 H	1	UNL1	0.1253
26 H	5.2053	-1.6682	-10.6714 H	1	UNL1	0.1385
27 H	4.5204	-3.0860	-11.4589 H	1	UNL1	0.1359
28 H	6.3000	-0.3709	-15.0142 H	1	UNL1	0.1097
29 H	2.2923	-2.9626	-12.5570 H	1	UNL1	0.1576
30 H	1.9936	-2.7415	-10.8241 H	1	UNL1	0.1548
31 H	1.2024	-1.6939	-12.0046 H	1	UNL1	0.1545
32 H	3.4562	3.0982	-13.6555 H	1	UNL1	0.1640
33 H	4.5132	3.9753	-12.5014 H	1	UNL1	0.1588
34 H	5.3822	1.5490	-16.3031 H	1	UNL1	0.1449
35 H	4.1028	1.7944	-15.1104 H	1	UNL1	0.1555
36 H	5.7869	2.0453	-14.6587 H	1	UNL1	0.1515
37 H	4.6029	-0.8144	-16.7967 H	1	UNL1	0.1459
38 H	4.4599	-2.0009	-15.4933 H	1	UNL1	0.1472
39 H	3.2874	-0.6896	-15.6228 H	1	UNL1	0.1517

@<TRIPOS>BOND
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 8    8   36   1
 9   28   14   1
10   14   17   1
11   12   19   1
12   32    9   1
13   24   16   1
14   17   19   1
15   17   16   1
16   17    2   1
17   19   20   1
18   19   18   1
19   16   25   1
20   16   15   1
21    9   33   1
22    9   21   2
23   29   13   1
24   11   20   1
25   20   21   1
26   20    1   1
27   31   13   1
28   21   22   1
29   13   18   1
30   13   30   1
31   18   15   1
32   18    1   1
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34   15   26   1
35    1   10   1
36    1   23   1
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Compound 29

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SMALL
MULLIKEN_CHARGES

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    2 C     4.4913   1.4051 -12.9262 C.3  1 UNL1    0.1658
    3 C     5.3103   2.7070 -12.7746 C.3  1 UNL1   -0.5169
    4 C     3.0068   1.7044 -13.0424 C.2  1 UNL1   -0.1178
    5 C     2.3313   2.5335 -12.2428 C.2  1 UNL1   -0.3713
    6 C     3.8219  -2.9669 -13.0719 C.2  1 UNL1    0.1280
    7 C     2.5067  -3.0969 -13.2796 C.2  1 UNL1   -0.4444
    8 C     4.7158  -4.1683 -12.9414 C.3  1 UNL1   -0.5111
    9 C     5.1661   1.2764 -15.4729 C.2  1 UNL1    0.1495
   10 C     4.3039   2.1889 -15.9333 C.2  1 UNL1   -0.4547
   11 C     6.3390   0.8461 -16.3187 C.3  1 UNL1   -0.5156
   12 H     6.1334   0.3684 -13.8275 H    1 UNL1    0.1378
   13 H     3.3306  -0.6842 -14.5598 H    1 UNL1    0.1456
   14 H     4.8706  -1.3840 -15.0705 H    1 UNL1    0.1327
   15 H     5.5982  -1.7898 -12.7697 H    1 UNL1    0.1281
   16 H     2.8790  -0.6618 -11.8325 H    1 UNL1    0.1448
   17 H     4.1301  -1.3914 -10.8158 H    1 UNL1    0.1290
   18 H     4.3034   1.0930 -10.7575 H    1 UNL1    0.1397
   19 H     5.7640   0.3865 -11.4563 H    1 UNL1    0.1339
   20 H     6.3927   2.5075 -12.7563 H    1 UNL1    0.1499
   21 H     5.1221   3.4007 -13.6068 H    1 UNL1    0.1665
   22 C     4.6831   0.5445 -11.6422 C.3  1 UNL1   -0.3086
   23 C     3.9744  -0.8125 -11.7472 C.3  1 UNL1   -0.2604
   24 C     4.5059  -1.6145 -12.9510 C.3  1 UNL1   -0.1147
   25 C     4.3881  -0.8033 -14.2599 C.3  1 UNL1   -0.2701
   26 H     5.0683   3.2420 -11.8425 H    1 UNL1    0.1534
   27 H     2.4650   1.1725 -13.8287 H    1 UNL1    0.1402
   28 H     1.2732   2.7057 -12.3534 H    1 UNL1    0.1473
   29 H     2.7926   3.0822 -11.4334 H    1 UNL1    0.1493
   30 H     2.0257  -4.0636 -13.3629 H    1 UNL1    0.1571
   31 H     1.8447  -2.2527 -13.3780 H    1 UNL1    0.1597
   32 H     5.2107  -4.1822 -11.9592 H    1 UNL1    0.1636
   33 H     4.1713  -5.1169 -13.0363 H    1 UNL1    0.1626
   34 H     5.4936  -4.1666 -13.7252 H    1 UNL1    0.1633
   35 H     4.4076   2.6461 -16.9036 H    1 UNL1    0.1556
   36 H     3.4398   2.5314 -15.3817 H    1 UNL1    0.1662
   37 H     6.3116  -0.2369 -16.5186 H    1 UNL1    0.1626
   38 H     6.3594   1.3606 -17.3024 H    1 UNL1    0.1635
   39 H     7.2947   1.0741 -15.8227 H    1 UNL1    0.1611
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    8    9   1  1
    9   14  25  1
   10   13  25  1
   11   25   1  1
   12   25  24  1
   13    1  12  1
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Compound 30

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SMALL
MULLIKEN_CHARGES

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    2 C    4.6275  -0.6908 -15.6962 C.3   1 UNL1   -0.3571
    3 C    3.9053  -0.4950 -14.3353 C.3   1 UNL1   -0.1361
    4 C    4.9218   0.6506 -14.0060 C.3   1 UNL1   -0.1346
    5 C    4.0370   0.4934 -11.3172 C.3   1 UNL1    0.1255
    6 C    4.5003   1.8558 -11.7691 C.3   1 UNL1   -0.3112
    7 C    4.4180   1.9124 -13.3114 C.3   1 UNL1   -0.2535
    8 C    2.5616   0.3052 -11.2299 C.3   1 UNL1   -0.4941
    9 C    4.9684  -0.4646 -11.1647 C.3   1 UNL1   -0.2786
   10 C    4.7141  -1.9345 -11.2229 C.3   1 UNL1   -0.2117
   11 C    4.8012  -2.3510 -12.7104 C.3   1 UNL1   -0.3030
   12 C    3.6901  -1.7409 -13.5286 C.2   1 UNL1    0.1423
   13 C    2.4897  -2.3333 -13.5696 C.2   1 UNL1   -0.4707
   14 C    4.3980   1.7790 -16.3078 C.3   1 UNL1   -0.5156
   15 C    6.6990   0.8691 -15.9077 C.3   1 UNL1   -0.5242
   16 H    5.8063   0.2592 -13.4625 H     1 UNL1    0.1431
   17 H    2.9034  -0.0274 -14.4988 H     1 UNL1    0.1360
   18 H    3.9938  -0.8762 -16.5595 H     1 UNL1    0.1426
   19 H    5.3900  -1.4788 -15.6819 H     1 UNL1    0.1458
   20 H    3.8899   2.6673 -11.3299 H     1 UNL1    0.1390
   21 H    5.5378   2.0569 -11.4363 H     1 UNL1    0.1412
   22 H    3.3740   2.1227 -13.6103 H     1 UNL1    0.1327
   23 H    5.0157   2.7749 -13.6674 H     1 UNL1    0.1320
   24 H    2.0887   0.4516 -12.2133 H     1 UNL1    0.1672
   25 H    2.2863  -0.7060 -10.9012 H     1 UNL1    0.1639
   26 H    2.1016   1.0211 -10.5386 H     1 UNL1    0.1552
   27 H    6.0272  -0.2035 -11.1581 H     1 UNL1    0.1438
   28 H    5.4650  -2.4935 -10.6332 H     1 UNL1    0.1259
   29 H    3.7273  -2.2060 -10.8014 H     1 UNL1    0.1363
   30 H    4.7604  -3.4554 -12.7882 H     1 UNL1    0.1405
   31 H    5.7923  -2.0515 -13.1230 H     1 UNL1    0.1459
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32 H	1.6573	-1.9599	-14.1424 H	1	UNL1	0.1550
33 H	2.2569	-3.2382	-13.0385 H	1	UNL1	0.1566
34 H	4.7143	2.8015	-16.0832 H	1	UNL1	0.1527
35 H	4.4843	1.6386	-17.3904 H	1	UNL1	0.1540
36 H	3.3324	1.7082	-16.0594 H	1	UNL1	0.1549
37 H	7.0919	1.8495	-15.6192 H	1	UNL1	0.1565
38 H	7.3083	0.1103	-15.4065 H	1	UNL1	0.1547
39 H	6.8568	0.7538	-16.9861 H	1	UNL1	0.1570

@<TRIPOS>BOND
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 3    18    2   1
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 7    15   37   1
 8    15    1   1
 9    15   38   1
10     2   19   1
11     2    1   1
12     2    3   1
13     1    4   1
14    17    3   1
15     3    4   1
16     3   12   1
17    32   13   1
18     4   16   1
19     4    7   1
20    23    7   1
21    22    7   1
22    13   12   2
23    13   33   1
24    12   11   1
25     7    6   1
26    31   11   1
27    30   11   1
28    11   10   1
29    24    8   1
30     6   21   1
31     6   20   1
32     6    5   1
33     5    8   1
34     5    9   1
35     8   25   1
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37    10    9   1
38    10   29   1
39    10   28   1
40     9   27   1
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Compound 31

@<TRIPOS>MOLECULE
compuesto_31.out
 39 41 0 0 0
SMALL
MULLIKEN_CHARGES

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1 C	5.4170	-1.3561	-15.8449 C.3	1	UNL1	-0.2662
2 C	3.9966	1.9975	-13.3650 C.3	1	UNL1	-0.0355
3 C	2.5816	-2.2878	-13.9787 C.2	1	UNL1	-0.4558
4 C	5.1569	-2.1360	-12.3390 C.3	1	UNL1	-0.5048
5 C	6.5844	0.5591	-12.6721 C.3	1	UNL1	-0.5206
6 C	3.2555	3.1583	-14.0410 C.3	1	UNL1	-0.4997
7 H	5.4819	-2.4558	-15.8909 H	1	UNL1	0.1297
8 H	5.7161	-0.9888	-16.8418 H	1	UNL1	0.1282

9 H	3.2851	-1.3142	-16.3187 H	1	UNL1	0.1227
10 H	7.1243	-0.1574	-15.2225 H	1	UNL1	0.1313
11 H	6.9007	-1.6310	-14.2752 H	1	UNL1	0.1344
12 H	4.2404	1.0170	-16.4963 H	1	UNL1	0.1275
13 H	2.8672	0.9522	-15.3985 H	1	UNL1	0.1393
14 H	5.5689	1.8553	-14.8476 H	1	UNL1	0.1189
15 H	4.3203	0.1647	-11.1511 H	1	UNL1	0.1332
16 H	2.8947	-0.7904	-11.5584 H	1	UNL1	0.1347
17 H	2.1801	0.7961	-13.2661 H	1	UNL1	0.1415
18 H	2.5250	1.6942	-11.7862 H	1	UNL1	0.1246
19 H	4.7236	2.4323	-12.6346 H	1	UNL1	0.1145
20 H	2.2857	-2.6827	-13.0217 H	1	UNL1	0.1560
21 H	1.9752	-2.6599	-14.7873 H	1	UNL1	0.1534
22 H	5.8623	-1.8200	-11.5654 H	1	UNL1	0.1501
23 H	4.4117	-2.7853	-11.8694 H	1	UNL1	0.1527
24 H	5.7074	-2.7549	-13.0582 H	1	UNL1	0.1567
25 H	7.1993	-0.2413	-12.2491 H	1	UNL1	0.1525
26 H	7.2636	1.2790	-13.1395 H	1	UNL1	0.1506
27 H	2.4577	2.7984	-14.7015 H	1	UNL1	0.1515
28 C	4.4977	-0.9290	-13.0331 C.3	1	UNL1	0.0984
29 C	6.3567	-0.8006	-14.7626 C.3	1	UNL1	-0.3065
30 C	3.5934	-1.4391	-14.1584 C.2	1	UNL1	0.0855
31 C	3.9697	-0.9214	-15.5358 C.3	1	UNL1	-0.0980
32 C	4.8113	1.1767	-14.3948 C.3	1	UNL1	-0.1272
33 C	3.9139	0.6174	-15.5219 C.3	1	UNL1	-0.2851
34 C	5.5742	0.0079	-13.6892 C.3	1	UNL1	0.1305
35 C	3.0024	1.1088	-12.5932 C.3	1	UNL1	-0.2811
36 C	3.6697	-0.1327	-11.9947 C.3	1	UNL1	-0.2916
37 H	6.0946	1.0699	-11.8343 H	1	UNL1	0.1580
38 H	2.7916	3.8177	-13.3019 H	1	UNL1	0.1470
39 H	3.9276	3.7699	-14.6505 H	1	UNL1	0.1485

@<TRIPOS>BOND
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 8   31   30   1
 9   33   13   1
10   33   32   1
11   10   29   1
12   14   32   1
13   21    3   1
14   29   11   1
15   29   34   1
16   27    6   1
17   39    6   1
18   32   34   1
19   32    2   1
20   30    3   2
21   30   28   1
22    6    2   1
23    6   38   1
24    3   20   1
25   34   28   1
26   34    5   1
27    2   19   1
28    2   35   1
29   17   35   1
30   26    5   1
31   24    4   1
32   28    4   1
33   28   36   1
34    5   25   1
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35	5	37	1
36	35	36	1
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38	4	23	1
39	4	22	1
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41	36	15	1

Compound 32

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compuesto_32.out
 39 40 0 0 0
SMALL
MULLIKEN_CHARGES

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   2 H     3.1962   2.6812 -14.4792 H    1 UNL1     0.1586
   3 H     6.4147   0.2791 -15.4278 H    1 UNL1     0.1638
   4 H     6.5905   2.0086 -15.7524 H    1 UNL1     0.1629
   5 H     7.1119   1.3496 -14.1958 H    1 UNL1     0.1640
   6 C     3.3163  -0.0245  -8.6058 C.3  1 UNL1    -0.2884
   7 C     3.8514  -1.2978  -9.2946 C.3  1 UNL1    -0.2693
   8 C     3.7570  -0.9710 -10.7724 C.2  1 UNL1    -0.0553
   9 C     3.8962  -2.0364 -11.8264 C.3  1 UNL1    -0.0226
  10 C     3.1164  -1.6625 -13.1071 C.3  1 UNL1    -0.2792
  11 C     3.8472  -0.6840 -14.0341 C.3  1 UNL1    -0.2705
  12 C     4.5333   0.5038 -13.3299 C.3  1 UNL1    -0.1024
  13 C     3.6494   1.1362 -12.2338 C.3  1 UNL1    -0.2763
  14 C     3.6300   0.3591 -10.9576 C.2  1 UNL1    -0.0533
  15 C     3.5337   1.1149  -9.6360 C.3  1 UNL1    -0.0364
  16 C     2.4217   2.1618  -9.5774 C.3  1 UNL1    -0.4877
  17 C     4.9675   1.5041 -14.3950 C.2  1 UNL1     0.1341
  18 C     3.4264  -3.4184 -11.3379 C.3  1 UNL1    -0.4914
  19 C     4.1889   2.4966 -14.8369 C.2  1 UNL1    -0.4557
  20 C     6.3341   1.2759 -14.9685 C.3  1 UNL1    -0.5134
  21 H     2.6111   1.2886 -12.5926 H    1 UNL1     0.1500
  22 H     4.0442   2.1541 -12.0201 H    1 UNL1     0.1448
  23 H     5.4578   0.1281 -12.8165 H    1 UNL1     0.1368
  24 H     3.1161  -0.3009 -14.7767 H    1 UNL1     0.1374
  25 H     4.6159  -1.2364 -14.6122 H    1 UNL1     0.1276
  26 H     2.1246  -1.2564 -12.8204 H    1 UNL1     0.1427
  27 H     2.9003  -2.5757 -13.6978 H    1 UNL1     0.1287
  28 H     4.9883  -2.1183 -12.0732 H    1 UNL1     0.1254
  29 H     3.2634  -2.1767  -8.9933 H    1 UNL1     0.1373
  30 H     4.9051  -1.5039  -9.0336 H    1 UNL1     0.1374
  31 H     3.7930   0.1764  -7.6375 H    1 UNL1     0.1290
  32 H     2.2330  -0.1503  -8.4161 H    1 UNL1     0.1384
  33 H     4.5177   1.6123  -9.4529 H    1 UNL1     0.1217
  34 H     2.3533   2.6000  -8.5708 H    1 UNL1     0.1484
  35 H     2.5969   2.9832 -10.2829 H    1 UNL1     0.1493
  36 H     1.4423   1.7262  -9.8202 H    1 UNL1     0.1550
  37 H     3.5311  -4.1759 -12.1240 H    1 UNL1     0.1472
  38 H     4.0198  -3.7684 -10.4842 H    1 UNL1     0.1491
  39 H     2.3670  -3.3650 -11.0405 H    1 UNL1     0.1556
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   7   19   17   2
   8   24   11   1
   9   25   11   1
  10   17   12   1
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13	27	10	1
14	12	23	1
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31	36	16	1
32	15	16	1
33	15	33	1
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39	6	32	1
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Compound 33

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 39 39 0 0 0
SMALL
MULLIKEN_CHARGES

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    2 C     3.1264   0.7519 -11.7333 C.3    1 UNL1     0.2366
    3 C     4.2607  -0.2245 -11.9679 C.2    1 UNL1    -0.2052
    4 C     4.1961  -1.5585 -11.9550 C.2    1 UNL1    -0.1420
    5 C     4.6240   1.4241 -14.8915 C.2    1 UNL1     0.0820
    6 C     5.2612   0.7959 -16.1114 C.3    1 UNL1    -0.2960
    7 C     5.3110   2.6751 -14.4265 C.3    1 UNL1    -0.5001
    8 H     6.2639   1.2403 -16.2787 H      1 UNL1     0.1401
    9 H     4.6637   1.0761 -17.0043 H      1 UNL1     0.1408
   10 H     6.1922  -1.0582 -16.7858 H      1 UNL1     0.1309
   11 H     4.4713  -1.2059 -16.4285 H      1 UNL1     0.1330
   12 H     3.3282  -2.1148 -11.6167 H      1 UNL1     0.1369
   13 H     6.4830  -0.6020 -14.1662 H      1 UNL1     0.1507
   14 H     3.0700   0.0035 -14.6179 H      1 UNL1     0.1526
   15 H     5.1826   0.2789 -12.2787 H      1 UNL1     0.1530
   16 H     1.8022   1.6320 -13.2579 H      1 UNL1     0.1422
   17 H     3.2462   2.5859 -12.9390 H      1 UNL1     0.1399
   18 H     6.2958  -2.0653 -12.2205 H      1 UNL1     0.1495
   19 H     5.2163  -3.4554 -12.2551 H      1 UNL1     0.1430
   20 H     4.2372  -3.1653 -15.7967 H      1 UNL1     0.1569
   21 H     4.2671  -4.1796 -14.3515 H      1 UNL1     0.1567
   22 H     3.1185  -2.8378 -14.4618 H      1 UNL1     0.1646
   23 H     3.4602   2.7808 -10.9296 H      1 UNL1     0.1509
   24 H     2.8936   1.6306  -9.7262 H      1 UNL1     0.1561
   25 H     4.5607   1.5751 -10.2751 H      1 UNL1     0.1571
   26 H     1.4964  -0.6603 -12.1144 H      1 UNL1     0.1565
   27 H     1.9339  -0.5183 -10.4057 H      1 UNL1     0.1546
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28 H	1.0061	0.7648	-11.1908 H	1	UNL1	0.1514
29 H	4.8062	3.1242	-13.5569 H	1	UNL1	0.1606
30 H	6.3441	2.4655	-14.1207 H	1	UNL1	0.1594
31 H	5.3408	3.4356	-15.2153 H	1	UNL1	0.1560
32 C	1.8179	0.0443	-11.3381 C.3	1	UNL1	-0.5257
33 C	3.5311	1.7368	-10.6097 C.3	1	UNL1	-0.5304
34 C	4.1464	-3.1484	-14.7029 C.3	1	UNL1	-0.4926
35 C	5.2956	-2.3971	-12.5608 C.3	1	UNL1	-0.3088
36 C	5.1333	-2.2279	-14.0590 C.2	1	UNL1	0.0931
37 C	3.5377	0.9277	-14.2785 C.2	1	UNL1	-0.2199
38 C	5.7470	-1.2144	-14.6887 C.2	1	UNL1	-0.2425
39 C	5.4107	-0.7384	-16.0674 C.3	1	UNL1	-0.2276

@<TRIPOS>BOND
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 8   20   34   1
 9   31    7   1
10    5    7   1
11    5   37   2
12   34   22   1
13   34   21   1
14   34   36   1
15   38   13   1
16   38   36   2
17   14   37   1
18    7   30   1
19    7   29   1
20   37    1   1
21   36   35   1
22   16    1   1
23    1   17   1
24    1    2   1
25   35   19   1
26   35   18   1
27   35    4   1
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Compound 34

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SMALL
MULLIKEN_CHARGES

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2 C	4.0344	-0.4267	-14.1411 C.3	1	UNL1	-0.2043
3 H	3.1581	3.9770	-14.6372 H	1	UNL1	0.1555
4 H	3.6786	3.2482	-16.1939 H	1	UNL1	0.1588
5 H	4.9602	-2.6956	-15.3506 H	1	UNL1	0.1580

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 6 H      6.4203  -2.7001 -14.3610 H    1 UNL1    0.1490
 7 H      6.5418  -2.9461 -16.1181 H    1 UNL1    0.1456
 8 H      7.2679  -0.6557 -15.4567 H    1 UNL1    0.1106
 9 H      4.8311  -1.0066 -17.2592 H    1 UNL1    0.1355
10 H      6.4409  -0.3652 -17.6428 H    1 UNL1    0.1276
11 H      5.5388   1.8069 -17.2930 H    1 UNL1    0.1263
12 H      4.0155   1.0744 -16.7516 H    1 UNL1    0.1388
13 H      5.6951   2.8253 -12.6654 H    1 UNL1    0.1413
14 H      4.0006   3.3478 -12.5897 H    1 UNL1    0.1430
15 H      5.1906   0.7454 -11.7908 H    1 UNL1    0.1305
16 H      3.7215   1.5263 -11.2257 H    1 UNL1    0.1275
17 H      2.3755   0.6561 -13.0719 H    1 UNL1    0.1493
18 H      3.4240  -0.5787 -15.0405 H    1 UNL1    0.1535
19 H      6.0746  -0.0053 -13.5353 H    1 UNL1    0.1203
20 H      6.4952   1.7958 -15.0934 H    1 UNL1    0.1312
21 C      4.6691  -1.8371 -11.9858 C.3  1 UNL1   -0.4809
22 C      2.3836  -2.0822 -13.0162 C.3  1 UNL1   -0.4941
23 C      3.6351  -1.2240 -12.8988 C.3  1 UNL1    0.1130
24 C      3.7710   3.2373 -15.1237 C.2  1 UNL1   -0.4683
25 C      6.0116  -2.3916 -15.3312 C.3  1 UNL1   -0.4874
26 C      6.1737  -0.8908 -15.5286 C.3  1 UNL1   -0.0449
27 C      5.6439  -0.3610 -16.8820 C.3  1 UNL1   -0.2899
28 C      5.1125   1.0622 -16.6042 C.3  1 UNL1   -0.2617
29 C      5.4650  -0.0226 -14.4598 C.3  1 UNL1   -0.0753
30 C      5.4534   1.3867 -15.1257 C.3  1 UNL1   -0.1366
31 C      4.5636   2.4052 -14.4440 C.2  1 UNL1    0.1394
32 C      4.6494   2.5150 -12.9372 C.3  1 UNL1   -0.3104
33 C      4.2612   1.2474 -12.1512 C.3  1 UNL1   -0.2236
34 C      3.3996   0.2895 -12.9479 C.3  1 UNL1   -0.2055
35 H      1.6179  -1.6303 -13.6739 H    1 UNL1    0.1544
36 H      2.6249  -3.0669 -13.4383 H    1 UNL1    0.1542
37 H      4.8802  -2.8847 -12.2940 H    1 UNL1    0.1562
38 H      5.6281  -1.2999 -11.9886 H    1 UNL1    0.1536
39 H      4.2979  -1.8597 -10.9521 H    1 UNL1    0.1538
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11   26   25   1
12   26   29   1
13    5   25   1
14   25    6   1
15   30   20   1
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25    2   23   1
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29   22   23   1
30   22    1   1
31   34   23   1
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Compound 35

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 39 41 0 0 0
SMALL
MULLIKEN_CHARGES

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      3 C        3.6139  -2.1325 -14.5769 C.3    1 UNL1      -0.2829
      4 H        5.9799  -0.4658 -14.0849 H      1 UNL1       0.1310
      5 C        5.3312  -1.4229 -16.3567 C.3    1 UNL1      -0.4972
      6 H        4.3023  -2.9906 -14.4955 H      1 UNL1       0.1321
      7 H        2.7180  -2.4904 -15.1194 H      1 UNL1       0.1265
      8 H        2.1717  -1.3479 -13.1210 H      1 UNL1       0.1370
      9 H        3.4045  -2.3775 -12.4120 H      1 UNL1       0.1335
     10 H        3.4908  -0.3853 -15.8725 H      1 UNL1       0.1168
     11 H        6.6120   0.7340 -10.7675 H      1 UNL1       0.1389
     12 H        5.2874   2.7978 -11.3414 H      1 UNL1       0.1331
     13 H        6.4616   2.4324 -12.6115 H      1 UNL1       0.1356
     14 H        3.9904   3.0341 -13.3408 H      1 UNL1       0.1176
     15 H        4.3620   1.7153 -15.3744 H      1 UNL1       0.1322
     16 H        6.0021   1.7545 -14.7078 H      1 UNL1       0.1324
     17 H        5.8074  -2.4348 -11.8941 H      1 UNL1       0.1637
     18 H        6.1869  -1.6234 -10.3674 H      1 UNL1       0.1550
     19 H        4.5307  -2.1343 -10.6964 H      1 UNL1       0.1601
     20 H        2.4083   0.9819 -14.7866 H      1 UNL1       0.1576
     21 H        1.3305   0.3523 -13.5182 H      1 UNL1       0.1514
     22 H        1.6188   2.1082 -13.6648 H      1 UNL1       0.1482
     23 H        2.0592   0.3674 -11.0640 H      1 UNL1       0.1513
     24 H        3.5413   1.2131 -10.5790 H      1 UNL1       0.1656
     25 H        2.1829   2.1438 -11.2563 H      1 UNL1       0.1486
     26 H        5.7081  -0.5523 -16.9105 H      1 UNL1       0.1503
     27 C        3.2837   1.0056 -12.7646 C.3    1 UNL1       0.1698
     28 C        2.7404   1.1985 -11.3436 C.3    1 UNL1      -0.5178
     29 C        2.0938   1.1161 -13.7379 C.3    1 UNL1      -0.5160
     30 C        5.4316  -1.7074 -11.1591 C.3    1 UNL1      -0.4905
     31 C        4.9688   1.4163 -14.4985 C.3    1 UNL1      -0.3054
     32 C        4.4015   2.0219 -13.1848 C.3    1 UNL1      -0.1065
     33 C        5.5316   2.0600 -12.1304 C.3    1 UNL1      -0.2618
     34 C        5.8100   0.7232 -11.4984 C.2    1 UNL1      -0.2451
     35 C        5.1308  -0.3967 -11.8112 C.2    1 UNL1       0.0529
     36 C        4.2830  -0.9691 -15.3415 C.3    1 UNL1      -0.0433
     37 C        4.9398  -0.1039 -14.2484 C.3    1 UNL1      -0.1130
     38 C        4.1006  -0.3331 -12.9310 C.3    1 UNL1       0.0278
     39 C        3.2511  -1.5943 -13.1736 C.3    1 UNL1      -0.2890
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     6   15   31    1
     7   36    3    1
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Compound 36

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SMALL
MULLIKEN_CHARGES

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      2 H      5.5614   1.6549 -13.9967 H     1 UNL1      0.1409
      3 H      4.2275   0.4632 -14.0446 H     1 UNL1      0.1543
      4 H      6.1054   0.9607 -11.6422 H     1 UNL1      0.1315
      5 H      6.3321  -0.3453 -12.7975 H     1 UNL1      0.1299
      6 H      4.9774  -0.5903 -10.4290 H     1 UNL1      0.1269
      7 H      1.9627  -1.4068 -10.1791 H     1 UNL1      0.1474
      8 H      1.8743   2.4584  -8.9839 H     1 UNL1      0.1446
      9 H      3.2875   1.9366  -8.0354 H     1 UNL1      0.1423
     10 H      3.7710   3.2553 -10.2289 H     1 UNL1      0.1316
     11 H      4.7034   1.7676  -9.9660 H     1 UNL1      0.1383
     12 H      4.2558   3.7350 -13.9610 H     1 UNL1      0.1573
     13 H      3.0718   4.0438 -12.6058 H     1 UNL1      0.1595
     14 H      5.7531  -2.3632 -11.8572 H     1 UNL1      0.1056
     15 H      1.0967  -1.1383  -7.9842 H     1 UNL1      0.1597
     16 H      2.0938  -0.0820  -6.9707 H     1 UNL1      0.1615
     17 H      0.5863   0.5382  -7.7014 H     1 UNL1      0.1615
     18 H      4.3688  -3.4130 -13.6544 H     1 UNL1      0.1456
     19 H      3.1870  -2.0903 -13.5640 H     1 UNL1      0.1505
     20 H      4.8575  -1.7720 -14.1044 H     1 UNL1      0.1477
     21 H      4.2708  -4.1214 -11.1966 H     1 UNL1      0.1445
     22 H      4.1231  -2.8723  -9.9418 H     1 UNL1      0.1519
     23 H      2.8458  -3.0726 -11.1765 H     1 UNL1      0.1521
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24 C	3.9352	-3.0847	-11.0091	C.3	1 UNL1	-0.4958
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26 C	1.4621	-0.1084	-7.8747	C.3	1 UNL1	-0.5055
27 H	2.5675	-0.3532	-12.2902	H	1 UNL1	0.1255
28 H	2.0810	1.8778	-11.5904	H	1 UNL1	0.1396
29 C	4.6660	-2.0991	-11.9332	C.3	1 UNL1	-0.0016
30 C	3.7439	3.3480	-13.1039	C.2	1 UNL1	-0.4695
31 C	3.6811	2.1508	-10.1614	C.3	1 UNL1	-0.2470
32 C	2.7541	1.7790	-8.9955	C.3	1 UNL1	-0.3012
33 C	2.2383	0.3649	-9.0750	C.2	1 UNL1	0.1010
34 C	2.4072	-0.4143	-10.1596	C.2	1 UNL1	-0.2846
35 C	3.8988	2.0882	-12.6779	C.2	1 UNL1	0.1168
36 C	3.1463	1.5600	-11.4790	C.3	1 UNL1	-0.1362
37 C	3.1516	0.0093	-11.4077	C.3	1 UNL1	-0.0544
38 C	4.5781	-0.6053	-11.4755	C.3	1 UNL1	-0.1128
39 C	5.5476	0.2715	-12.3123	C.3	1 UNL1	-0.2653

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  8     1   35   1
  9     1   39   1
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 11    30   13   1
 12     5   39   1
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 35    33   26   1
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Compound 37

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SMALL
MULLIKEN_CHARGES


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3 H	5.4458	-3.9741	-13.2329	H	1 UNL1	0.1490
4 H	2.3682	0.4188	-8.3135	H	1 UNL1	0.1578
5 H	2.5448	-1.0771	-9.2360	H	1 UNL1	0.1633
6 H	0.9668	-0.2863	-9.1259	H	1 UNL1	0.1604
7 H	6.1081	-1.6088	-12.8720	H	1 UNL1	0.1170
8 H	5.5547	4.3862	-13.7986	H	1 UNL1	0.1573
9 H	5.3531	3.4409	-15.3102	H	1 UNL1	0.1556
10 H	3.2969	3.7582	-11.2808	H	1 UNL1	0.1308
11 H	2.7330	2.5176	-12.4085	H	1 UNL1	0.1427
12 H	3.3919	2.2013	-9.4362	H	1 UNL1	0.1461
13 H	1.8361	0.8250	-12.5626	H	1 UNL1	0.1536
14 H	0.7936	-0.2545	-11.6205	H	1 UNL1	0.1392
15 H	5.2834	1.5308	-11.5411	H	1 UNL1	0.1556
16 H	5.5175	3.3007	-11.6580	H	1 UNL1	0.1434
17 H	2.6767	-1.9184	-11.4036	H	1 UNL1	0.1346
18 H	2.2310	-1.6046	-13.0813	H	1 UNL1	0.1296
19 H	4.4985	-0.0310	-11.6921	H	1 UNL1	0.1545
20 H	3.9948	-0.8394	-14.6374	H	1 UNL1	0.1322
21 H	4.5956	1.2872	-15.3241	H	1 UNL1	0.1481
22 H	4.5099	-2.9207	-14.2972	H	1 UNL1	0.1477
23 H	4.5262	-2.7771	-10.4855	H	1 UNL1	0.1500
24 H	6.1808	-3.1651	-10.9378	H	1 UNL1	0.1493
25 H	5.7736	-1.5379	-10.3856	H	1 UNL1	0.1500
26 C	5.4162	-2.3824	-10.9838	C.3	1 UNL1	-0.4976
27 C	4.6852	-3.1842	-13.2500	C.3	1 UNL1	-0.4936
28 C	2.0440	-0.1007	-9.2229	C.3	1 UNL1	-0.5043
29 C	5.1402	-1.9679	-12.4334	C.3	1 UNL1	-0.0014
30 C	5.2982	3.4308	-14.2310	C.2	1 UNL1	-0.4449
31 C	3.4261	2.6911	-11.5554	C.3	1 UNL1	-0.2221
32 C	3.0484	1.8209	-10.3976	C.2	1 UNL1	-0.2743
33 C	2.3533	0.6743	-10.4684	C.2	1 UNL1	0.1109
34 C	1.8481	0.0629	-11.7476	C.3	1 UNL1	-0.3064
35 C	4.9498	2.3520	-13.5109	C.2	1 UNL1	0.1399
36 C	4.8832	2.4564	-12.0095	C.3	1 UNL1	-0.3015
37 C	2.6965	-1.1411	-12.1914	C.3	1 UNL1	-0.2432
38 C	4.1627	-0.7527	-12.4863	C.3	1 UNL1	-0.1242
39 C	4.2577	-0.1235	-13.8494	C.2	1 UNL1	-0.1159

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Compound 38

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SMALL
MULLIKEN_CHARGES

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      3 H      5.5319  -1.1660 -17.8354 H      1 UNL1      0.1558
      4 H      2.5413  -0.9626 -16.1132 H      1 UNL1      0.1634
      5 H      3.1736  -0.7616 -17.7583 H      1 UNL1      0.1632
      6 H      2.7441   0.6749 -16.7816 H      1 UNL1      0.1632
      7 H      2.3462  -2.2410 -12.3431 H      1 UNL1      0.1488
      8 H      2.2354  -2.3711 -10.5802 H      1 UNL1      0.1462
      9 H      3.7159  -2.8802 -11.4036 H      1 UNL1      0.1494
     10 H      5.7594  -2.1025 -11.7054 H      1 UNL1      0.1497
     11 H      6.1965  -0.6574 -10.7621 H      1 UNL1      0.1519
     12 H      6.7539  -0.8392 -12.4310 H      1 UNL1      0.1555
     13 H      4.2823   3.1581 -11.6351 H      1 UNL1      0.1403
     14 H      3.0722   1.7132  -9.7487 H      1 UNL1      0.1371
     15 H      2.0318   2.4564 -10.9889 H      1 UNL1      0.1313
     16 H      1.5017   0.0020 -10.5847 H      1 UNL1      0.1287
     17 H      1.8855   0.3842 -12.2823 H      1 UNL1      0.1378
     18 H      3.9214  -0.6504 -10.2083 H      1 UNL1      0.1241
     19 H      6.9521   1.5832 -12.5264 H      1 UNL1      0.1422
     20 H      5.8940   2.7813 -13.2905 H      1 UNL1      0.1369
     21 H      4.6917  -1.6784 -13.9283 H      1 UNL1      0.1445
     22 H      3.1565  -0.8010 -13.8061 H      1 UNL1      0.1383
     23 H      3.9777   1.2104 -14.7489 H      1 UNL1      0.1379
     24 H      6.4172   1.6190 -15.2285 H      1 UNL1      0.1316
     25 H      6.8227   0.1186 -14.3657 H      1 UNL1      0.1350
     26 C      5.6321  -0.7390 -16.8508 C.2    1 UNL1     -0.4544
     27 C      3.1992  -0.3306 -16.7350 C.3    1 UNL1     -0.5117
     28 C      4.5848  -0.2638 -16.1648 C.2    1 UNL1      0.1332
     29 C      2.9197  -2.1209 -11.4091 C.3    1 UNL1     -0.4872
     30 C      5.8959  -1.0107 -11.7637 C.3    1 UNL1     -0.5094
     31 C      4.0562   2.0892 -11.6046 C.2    1 UNL1     -0.2391
     32 C      2.8327   1.7034 -10.8447 C.3    1 UNL1     -0.2423
     33 C      2.3180   0.3243 -11.2619 C.3    1 UNL1     -0.2839
     34 C      3.4707  -0.6983 -11.2380 C.3    1 UNL1     -0.0701
     35 C      6.0004   1.6939 -13.0873 C.3    1 UNL1     -0.2870
     36 C      4.8453   1.2089 -12.2398 C.2    1 UNL1      0.0116
     37 C      4.6058  -0.2975 -12.2424 C.3    1 UNL1      0.1436
     38 C      4.2542  -0.6858 -13.7072 C.3    1 UNL1     -0.3119
     39 C      4.6925   0.3449 -14.7757 C.3    1 UNL1     -0.1058
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Compound 39

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SMALL
MULLIKEN_CHARGES

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3 H	6.2851	-0.8671	-18.3277	H	1	UNL1	0.1621
4 H	3.5218	2.9773	-11.4651	H	1	UNL1	0.1278
5 H	2.2319	1.8377	-11.8885	H	1	UNL1	0.1374
6 H	4.4045	1.5972	-9.7206	H	1	UNL1	0.1354
7 H	2.6326	1.4031	-9.5563	H	1	UNL1	0.1324
8 H	3.6879	-0.8480	-9.3967	H	1	UNL1	0.1401
9 H	4.5569	3.0981	-13.7163	H	1	UNL1	0.1283
10 H	3.2428	2.1144	-14.3904	H	1	UNL1	0.1338
11 H	5.2407	1.2566	-12.2051	H	1	UNL1	0.1299
12 H	5.8461	-0.8169	-13.3438	H	1	UNL1	0.1436
13 H	4.6220	-1.8903	-14.0695	H	1	UNL1	0.1405
14 H	3.9124	-0.1159	-15.6458	H	1	UNL1	0.1322
15 H	5.2402	2.0007	-15.8715	H	1	UNL1	0.1270
16 H	6.2807	1.5183	-14.5128	H	1	UNL1	0.1388
17 C	4.0179	-2.4610	-11.4905	C.3	1	UNL1	-0.4864
18 C	2.3824	-0.4428	-13.3956	C.3	1	UNL1	-0.4993
19 C	7.0557	-1.2406	-15.8506	C.2	1	UNL1	-0.4492
20 C	5.5313	-0.4551	-17.6353	C.3	1	UNL1	-0.5103
21 C	5.9079	-0.6373	-16.1860	C.2	1	UNL1	0.1275

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22 C    3.2927   1.8958  -11.5702 C.3   1 UNL1   -0.2854
23 C    3.4960   1.1878  -10.2214 C.3   1 UNL1   -0.2388
24 C    3.6795  -0.2988  -10.3456 C.2   1 UNL1   -0.2347
25 C    3.8550  -0.9640  -11.4997 C.2   1 UNL1    0.0227
26 C    4.2508   2.0517  -13.9320 C.3   1 UNL1   -0.2812
27 C    4.9292  -0.0548  -15.1792 C.3   1 UNL1   -0.1014
28 H    1.6176  -0.1833  -12.6437 H     1 UNL1    0.1557
29 H    3.2556  -2.9485  -12.1231 H     1 UNL1    0.1596
30 H    5.0206  -2.7533  -11.8552 H     1 UNL1    0.1608
31 H    3.9024  -2.8918  -10.4826 H     1 UNL1    0.1537
32 H    7.7368  -1.6307  -16.6041 H     1 UNL1    0.1568
33 H    2.1765   0.1652  -14.2896 H     1 UNL1    0.1507
34 H    2.2042  -1.4968  -13.6750 H     1 UNL1    0.1479
35 H    5.4193   0.6130  -17.8730 H     1 UNL1    0.1626
36 H    7.3734  -1.3714  -14.8356 H     1 UNL1    0.1583
37 C    4.2001   1.2454  -12.6248 C.3   1 UNL1   -0.0956
38 C    3.8152  -0.2467  -12.8526 C.3   1 UNL1    0.1415
39 C    4.8563  -0.8302  -13.8450 C.3   1 UNL1   -0.3210
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12   27   39   1
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14    1   26   1
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Compound 40

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SMALL
MULLIKEN_CHARGES
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      2 C      4.7603    1.7249  -12.8450 C.3    1 UNL1     -0.1215
      3 C      4.6807    0.2122  -12.4634 C.3    1 UNL1     -0.0720
      4 C      5.0509   -0.7456  -13.6258 C.3    1 UNL1     -0.1299
      5 C      4.2716   -0.3879  -14.8956 C.3    1 UNL1     -0.2476
      6 H      2.2356    0.2989   -8.7224 H      1 UNL1      0.1597
      7 H      1.1597    1.1986   -9.8233 H      1 UNL1      0.1625
      8 H      6.2553   -4.0507  -13.5097 H      1 UNL1      0.1496
      9 H      6.3226   -2.9268  -14.8827 H      1 UNL1      0.1512
     10 H      7.1922   -2.5528  -13.3735 H      1 UNL1      0.1456
     11 H      3.7542   -4.0458  -13.3131 H      1 UNL1      0.1453
     12 H      2.8242   -2.5414  -13.4220 H      1 UNL1      0.1503
     13 H      3.7446   -3.1248  -14.8261 H      1 UNL1      0.1500
     14 C      4.6348    1.0355  -15.3293 C.3    1 UNL1     -0.3171
     15 H      1.3938   -0.5519  -10.0342 H      1 UNL1      0.1589
     16 H      5.0261   -2.3287  -12.1314 H      1 UNL1      0.1163
     17 H      3.5263    4.0147  -13.9217 H      1 UNL1      0.1588
     18 H      3.4703    3.4434  -15.6279 H      1 UNL1      0.1568
     19 H      4.6192    3.5652  -11.6505 H      1 UNL1      0.1270
     20 H      3.0425    2.8716  -12.1161 H      1 UNL1      0.1483
     21 H      4.8495    1.6669   -9.9372 H      1 UNL1      0.1445
     22 H      3.3489    2.6033   -9.7139 H      1 UNL1      0.1386
     23 H      2.8549   -0.9955  -11.9603 H      1 UNL1      0.1517
     24 H      6.1370   -0.5155  -13.8480 H      1 UNL1      0.1252
     25 H      3.1787   -0.4599  -14.7190 H      1 UNL1      0.1444
     26 H      4.5260   -1.0910  -15.7146 H      1 UNL1      0.1276
     27 H      4.1174    1.2716  -16.2826 H      1 UNL1      0.1446
     28 H      5.7222    1.1037  -15.5499 H      1 UNL1      0.1451
     29 C      3.7652   -3.0234  -13.7281 C.3    1 UNL1     -0.4900
     30 C      6.2656   -2.9810  -13.7829 C.3    1 UNL1     -0.5010
     31 C      1.9045    0.3857   -9.7696 C.3    1 UNL1     -0.4949
     32 H      5.4879    0.0595  -11.6930 H      1 UNL1      0.1216
     33 H      5.8535    1.9838  -12.8420 H      1 UNL1      0.1284
     34 C      5.0104   -2.2574  -13.2480 C.3    1 UNL1      0.0006
     35 C      3.7452    3.2121  -14.6137 C.2    1 UNL1     -0.4754
     36 C      4.0702    2.6106  -11.7715 C.3    1 UNL1     -0.2587
     37 C      3.8769    1.9202  -10.4079 C.3    1 UNL1     -0.2959
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Compound 41

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SMALL
MULLIKEN_CHARGES

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   3 H      5.5867  -0.0075 -17.2526 H      1 UNL1    0.1634
   4 H      5.3642   1.7061 -17.6513 H      1 UNL1    0.1627
   5 H      6.8039   1.1915 -16.7355 H      1 UNL1    0.1623
   6 C      5.4107   0.2720 -14.4371 C.3    1 UNL1   -0.1127
   7 H      2.8580  -1.6457  -9.4925 H      1 UNL1    0.1361
   8 H      5.6039  -1.2583 -10.8326 H      1 UNL1    0.1389
   9 H      4.6500  -2.7583 -10.7542 H      1 UNL1    0.1314
  10 H      5.9877   0.4892 -12.3363 H      1 UNL1    0.1356
  11 H      5.1774   1.9017 -12.9910 H      1 UNL1    0.1384
  12 H      5.2876  -1.6597 -15.4580 H      1 UNL1    0.1237
  13 H      5.8734  -1.9939 -13.0151 H      1 UNL1    0.1373
  14 H      4.5016  -2.9798 -13.5352 H      1 UNL1    0.1350
  15 H      3.7082  -1.0028 -14.9697 H      1 UNL1    0.1405
  16 H      6.5214   0.1566 -14.5203 H      1 UNL1    0.1254
  17 C      2.5089  -1.9050 -12.3212 C.3    1 UNL1   -0.5229
  18 H      3.0241   0.4531 -13.1360 H      1 UNL1    0.1430
  19 C      5.7222   1.0173 -16.8626 C.3    1 UNL1   -0.5130
  20 C      4.0007   2.1050 -15.4566 C.2    1 UNL1   -0.4529
  21 C      4.9830   1.2020 -15.5650 C.2    1 UNL1    0.1335
  22 C      3.0373   2.4049 -11.2697 C.3    1 UNL1   -0.4976
  23 C      3.4625   0.9651 -11.1204 C.2    1 UNL1    0.0663
  24 C      3.4319   0.3711  -9.9186 C.2    1 UNL1   -0.2472
  25 C      3.7914  -1.0612  -9.6822 C.3    1 UNL1   -0.2258
  26 C      4.5685  -1.6581 -10.8630 C.3    1 UNL1   -0.3208
  27 C      5.1534   0.7950 -13.0028 C.3    1 UNL1   -0.2748
  28 C      3.8458   0.2453 -12.3977 C.3    1 UNL1   -0.1433
  29 C      3.9305  -1.3070 -12.2297 C.3    1 UNL1    0.1923
  30 C      4.8128  -1.9314 -13.3490 C.3    1 UNL1   -0.3236
  31 C      4.7632  -1.1167 -14.6453 C.3    1 UNL1   -0.2540
  32 H      4.4082  -1.1538  -8.7630 H      1 UNL1    0.1282
  33 H      3.1107   0.9315  -9.0357 H      1 UNL1    0.1410
  34 H      2.6732   2.8336 -10.3284 H      1 UNL1    0.1554
  35 H      3.8795   3.0399 -11.5993 H      1 UNL1    0.1616
  36 H      2.2244   2.5026 -12.0054 H      1 UNL1    0.1596
  37 H      2.0865  -1.7873 -13.3339 H      1 UNL1    0.1503
  38 H      2.5127  -2.9829 -12.0907 H      1 UNL1    0.1491
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Compound 42

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MULLIKEN_CHARGES

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    3 C     4.1321   0.1515 -11.0559 C.2   1 UNL1     0.0736
    4 C     3.0423   1.1879 -11.1834 C.3   1 UNL1    -0.2915
    5 C     3.3155   2.1199 -12.3821 C.3   1 UNL1    -0.2550
    6 C     4.6307  -0.1889  -9.6834 C.3   1 UNL1    -0.4938
    7 C     4.7586   3.5973 -14.5884 C.3   1 UNL1    -0.4808
    8 H     2.8510  -0.3545 -13.4444 H     1 UNL1     0.1339
    9 C     4.6403  -2.3322 -14.6269 C.3   1 UNL1     0.0015
   10 C     4.9468  -2.9949 -15.9859 C.3   1 UNL1    -0.4972
   11 C     3.3702  -2.9855 -14.0482 C.3   1 UNL1    -0.4965
   12 H     6.5055   1.8966 -15.6502 H     1 UNL1     0.1371
   13 H     4.9972   1.4238 -16.4866 H     1 UNL1     0.1386
   14 H     6.5287  -0.1336 -14.2824 H     1 UNL1     0.1412
   15 H     6.3122  -0.5837 -15.9962 H     1 UNL1     0.1264
   16 H     3.7792  -0.5983 -15.5820 H     1 UNL1     0.1283
   17 H     5.3456  -1.2169 -12.1435 H     1 UNL1     0.1502
   18 H     2.0755   0.6510 -11.3125 H     1 UNL1     0.1437
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21 H	3.9819	2.9357	-12.0188	H	1	UNL1	0.1427
22 H	5.4081	-0.9730	-9.6990	H	1	UNL1	0.1590
23 H	5.0680	0.7048	-9.1988	H	1	UNL1	0.1620
24 H	3.7968	-0.5556	-9.0544	H	1	UNL1	0.1592
25 H	4.0280	4.1194	-13.9419	H	1	UNL1	0.1538
26 H	5.7678	3.9706	-14.3266	H	1	UNL1	0.1579
27 H	4.5361	3.9076	-15.6274	H	1	UNL1	0.1549
28 H	5.4930	-2.5624	-13.9431	H	1	UNL1	0.1122
29 H	5.9187	-2.6745	-16.4036	H	1	UNL1	0.1462
30 H	4.9983	-4.0978	-15.8893	H	1	UNL1	0.1478
31 H	4.1628	-2.7670	-16.7298	H	1	UNL1	0.1502
32 H	3.1727	-2.6679	-13.0067	H	1	UNL1	0.1550
33 H	2.4819	-2.7409	-14.6575	H	1	UNL1	0.1490
34 H	3.4621	-4.0890	-14.0233	H	1	UNL1	0.1461
35 C	4.7106	2.0967	-14.4734	C.2	1	UNL1	0.0069
36 C	4.0084	1.4299	-13.5391	C.2	1	UNL1	-0.0529
37 C	3.9381	-0.0856	-13.4934	C.3	1	UNL1	-0.0660
38 C	4.5059	-0.7897	-14.7496	C.3	1	UNL1	-0.1214
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Compound 43

@<TRIPOS>MOLECULE

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    3 C      3.2133  -0.6664 -12.5161 C.3   1 UNL1      -0.2072
    4 H      6.3369   1.7435 -14.2169 H     1 UNL1       0.1364
    5 H      5.3703   1.9768 -15.7015 H     1 UNL1       0.1341
    6 H      2.8445   3.3989 -11.4673 H     1 UNL1       0.1410
    7 H      1.9901   2.2136 -12.4751 H     1 UNL1       0.1532
    8 H      4.3179   1.3029 -10.6727 H     1 UNL1       0.1379
    9 H      2.7838   1.6605  -9.9376 H     1 UNL1       0.1265
   10 H      2.4901  -1.0984 -13.2277 H     1 UNL1       0.1708
   11 H      1.5386   0.0297 -11.1848 H     1 UNL1       0.1456
   12 O      3.8823  -1.5116 -15.0971 O.3   1 UNL1      -0.5900
   13 C      5.7475  -2.2332 -13.7754 C.3   1 UNL1      -0.5798
   14 H      3.3265   1.1846 -14.5939 H     1 UNL1       0.1555
   15 H      5.2375   0.0568 -12.4393 H     1 UNL1       0.1417
   16 C      4.6361  -1.4243 -10.3842 C.3   1 UNL1      -0.4852
   17 C      2.4461  -2.5403 -10.9086 C.3   1 UNL1      -0.4942
   18 C      3.3290  -1.3276 -11.1327 C.3   1 UNL1       0.1183
   19 C      4.6977   3.6225 -13.2204 C.2   1 UNL1      -0.4668
   20 C      4.9896  -1.0256 -14.3148 C.3   1 UNL1       0.3965
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   22 C      5.5012   1.3297 -14.8206 C.3   1 UNL1      -0.2519
   23 C      4.4260  -0.0932 -13.2026 C.3   1 UNL1      -0.1164
   24 C      4.2262   1.2646 -13.9336 C.3   1 UNL1      -0.1230
   25 C      4.0299   2.4763 -13.0467 C.2   1 UNL1       0.1223
   26 C      2.9627   2.4124 -11.9764 C.3   1 UNL1      -0.3047
   27 H      6.9134  -0.2972 -15.0828 H     1 UNL1       0.1459
   28 H      5.6231  -0.3065 -16.2972 H     1 UNL1       0.1502
   29 H      5.4438   3.8135 -13.9627 H     1 UNL1       0.1574
   30 H      4.5392   4.4907 -12.6089 H     1 UNL1       0.1553
   31 H      2.1959  -2.6378  -9.8379 H     1 UNL1       0.1560
   32 H      1.4891  -2.4709 -11.4518 H     1 UNL1       0.1551
   33 H      2.9437  -3.4536 -11.2834 H     1 UNL1       0.1581
   34 H      5.1922  -2.3175 -10.6451 H     1 UNL1       0.1518
   35 H      5.2998  -0.5644 -10.5667 H     1 UNL1       0.1560
   36 H      4.4660  -1.5187  -9.3101 H     1 UNL1       0.1559
   37 H      6.5717  -1.9151 -13.1225 H     1 UNL1       0.1665
   38 H      5.0751  -2.8655 -13.1738 H     1 UNL1       0.1825
   39 H      6.1452  -2.8521 -14.5987 H     1 UNL1       0.1598
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Compound 44

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SMALL
MULLIKEN_CHARGES

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     3 H     5.0590   1.1382 -16.9501 H     1 UNL1    0.1456
     4 H     2.3909  -1.3815 -11.9023 H     1 UNL1    0.1352
     5 H     4.1591  -1.4042 -11.5713 H     1 UNL1    0.1413
     6 C     5.9724  -2.8573 -12.9885 C.3   1 UNL1   -0.5320
     7 H     6.7007  -1.7508 -15.3483 H     1 UNL1    0.1383
     8 H     2.4453   0.6249 -13.0947 H     1 UNL1    0.1372
     9 H     5.5037   0.3229 -13.4018 H     1 UNL1    0.1407
    10 C     2.6142   2.0849 -10.9048 C.3   1 UNL1   -0.5232
    11 C     4.7206   0.7703 -10.3925 C.3   1 UNL1   -0.5149
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    13 O     5.0738  -3.1324 -15.2993 O.3   1 UNL1   -0.4897
    14 C     4.6271   2.1560 -12.5456 C.3   1 UNL1   -0.3553
    15 C     3.8089   1.3413 -11.4930 C.3   1 UNL1    0.1891
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    17 C     5.0077  -2.3173 -14.0155 C.3   1 UNL1    0.2800
    18 C     5.6028  -1.7916 -15.2758 C.3   1 UNL1    0.0348
    19 C     4.8769  -0.8694 -16.2361 C.3   1 UNL1   -0.2817
    20 C     5.1620   0.6096 -15.9891 C.3   1 UNL1   -0.3070
    21 C     4.2654   1.2243 -14.9441 C.2   1 UNL1    0.1173
    22 C     4.5851   0.9360 -13.5057 C.3   1 UNL1   -0.1311
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    27 H     3.1891  -3.0520 -13.3347 H     1 UNL1    0.1524
    28 H     4.0553   3.0126 -12.9483 H     1 UNL1    0.1526
    29 H     5.6303   2.4672 -12.2117 H     1 UNL1    0.1436
    30 H     2.9949   2.1974 -16.3523 H     1 UNL1    0.1579
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    32 H     4.1507   0.0796  -9.7659 H     1 UNL1    0.1535
    33 H     5.5876   0.2469 -10.8124 H     1 UNL1    0.1535
    34 H     5.1515   1.5719  -9.7339 H     1 UNL1    0.1570
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36 H	1.9921	1.4078	-10.3111 H	1 UNL1	0.1539
37 H	2.9944	2.8845	-10.2170 H	1 UNL1	0.1601
38 H	6.1270	-2.1603	-12.1754 H	1 UNL1	0.1649
39 H	5.5844	-3.8026	-12.5789 H	1 UNL1	0.1756
40 H	6.9907	-3.0795	-13.3586 H	1 UNL1	0.1730

@<TRIPOS>BOND
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 7   20   2  1
 8   20  21  1
 9    7  18  1
10   12  21  2
11   12  31  1
12   13  18  1
13   13  17  1
14   18  17  1
15   21  22  1
16   26  16  1
17   17  16  1
18   17   6  1
19   16  27  1
20   16  23  1
21   22   9  1
22   22   1  1
23   22  14  1
24   40   6  1
25    8   1  1
26    6  39  1
27    6  38  1
28   28  14  1
29    1  23  1
30    1  15  1
31   14  29  1
32   14  15  1
33   23   4  1
34   23   5  1
35   35  10  1
36   15  10  1
37   15  11  1
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39   10  37  1
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42   11  34  1
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Compound 45

@<TRIPOS>MOLECULE
compuesto_45.out
 42 43 0 0 0
SMALL
MULLIKEN_CHARGES

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1 H	6.3079	2.4454	-11.1006 H	1 UNL1	0.1494
2 H	4.6247	2.5554	-10.5697 H	1 UNL1	0.1550
3 H	5.3956	3.9228	-11.4146 H	1 UNL1	0.1485
4 C	4.2480	0.3540	-14.2557 C.3	1 UNL1	-0.2469
5 C	3.7106	-1.0780	-14.2576 C.3	1 UNL1	-0.3665
6 C	4.5134	-2.0044	-13.3314 C.3	1 UNL1	0.4009
7 C	4.3645	-1.5363	-11.8559 C.3	1 UNL1	-0.1538
8 C	4.1829	0.0190	-11.7307 C.3	1 UNL1	-0.0598
9 C	4.8379	0.7959	-12.8983 C.3	1 UNL1	-0.1311

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10 C      3.2529  -2.2985 -11.0981 C.3   1 UNL1    -0.2401
11 C      2.6491  -1.4993  -9.9275 C.3   1 UNL1    -0.3021
12 C      2.0506  -0.2405 -10.5184 C.2   1 UNL1     0.0851
13 C      2.7596   0.4241 -11.4345 C.2   1 UNL1    -0.2655
14 C      4.8205   2.3469 -12.7541 C.3   1 UNL1     0.0002
15 H      4.7565   0.2984 -10.8008 H     1 UNL1     0.1246
16 C      0.6839   0.1629 -10.0783 C.3   1 UNL1    -0.4986
17 H      5.3258  -1.7806 -11.3353 H     1 UNL1     0.1267
18 O      3.9309  -3.3226 -13.4407 O.3   1 UNL1    -0.5985
19 C      5.9735  -2.1763 -13.7810 C.3   1 UNL1    -0.5815
20 C      5.6797   3.0169 -13.8485 C.3   1 UNL1    -0.4996
21 C      5.3151   2.8291 -11.3786 C.3   1 UNL1    -0.4989
22 H      5.0384   0.4573 -15.0185 H     1 UNL1     0.1233
23 H      3.4276   1.0252 -14.5751 H     1 UNL1     0.1321
24 H      3.7320  -1.4743 -15.2810 H     1 UNL1     0.1331
25 H      2.6529  -1.0969 -13.9262 H     1 UNL1     0.1672
26 H      5.9199   0.4981 -12.8839 H     1 UNL1     0.1219
27 H      2.4073  -2.5344 -11.7775 H     1 UNL1     0.1536
28 H      3.6470  -3.2738 -10.7611 H     1 UNL1     0.1346
29 H      1.8837  -2.0980  -9.3951 H     1 UNL1     0.1392
30 H      3.4260  -1.2467  -9.1834 H     1 UNL1     0.1425
31 H      2.3688   1.3138 -11.9151 H     1 UNL1     0.1492
32 H      3.7679   2.7001 -12.8862 H     1 UNL1     0.1146
33 H     -0.0636  -0.6227 -10.2359 H     1 UNL1     0.1616
34 H      0.6673   0.3868  -8.9900 H     1 UNL1     0.1614
35 H      0.3388   1.0550 -10.6311 H     1 UNL1     0.1591
36 H      4.1036  -3.6759 -14.3365 H     1 UNL1     0.3105
37 H      6.5429  -1.2477 -13.6276 H     1 UNL1     0.1706
38 H      6.4819  -2.9418 -13.1781 H     1 UNL1     0.1692
39 H      6.0367  -2.5008 -14.8387 H     1 UNL1     0.1605
40 H      5.6607   4.1152 -13.6977 H     1 UNL1     0.1501
41 H      6.7283   2.6964 -13.7930 H     1 UNL1     0.1488
42 H      5.3291   2.7782 -14.8691 H     1 UNL1     0.1492
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  7     5    4   1
  8     5   25   1
  9     5    6   1
 10     4    9   1
 11    20   41   1
 12    20   40   1
 13    20   14   1
 14    19   37   1
 15    19    6   1
 16    19   38   1
 17    18    6   1
 18     6    7   1
 19     9   26   1
 20     9   14   1
 21     9    8   1
 22    32   14   1
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 26     7   17   1
 27     7   10   1
 28    27   10   1
 29     8   13   1
 30     8   15   1
 31    13   12   2
 32     3   21   1
```

33	21	1	1
34	21	2	1
35	10	28	1
36	10	11	1
37	35	16	1
38	12	16	1
39	12	11	1
40	33	16	1
41	16	34	1
42	11	29	1
43	11	30	1

Compound 46

@<TRIPOS>MOLECULE
compuesto_46.out
 42 43 0 0 0
SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM
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   1 H     4.7139   2.5515 -10.8014 H     1 UNL1     0.1560
   2 H     6.3936   2.4346 -11.4004 H     1 UNL1     0.1497
   3 H     4.2102  -3.6562 -14.6496 H     1 UNL1     0.3103
   4 C     4.3290   0.3753 -14.5261 C.3   1 UNL1    -0.2472
   5 C     4.8900   2.3576 -13.0040 C.3   1 UNL1    -0.0007
   6 H     4.8460   0.2858 -11.0732 H     1 UNL1     0.1248
   7 C     0.7770   0.1192 -10.3403 C.3   1 UNL1    -0.4987
   8 C     6.0697  -2.1517 -14.0863 C.3   1 UNL1    -0.5812
   9 C     5.7470   3.0415 -14.0936 C.3   1 UNL1    -0.5000
  10 C     5.3917   2.8258 -11.6262 C.3   1 UNL1    -0.4983
  11 H     5.4252  -1.7834 -11.6325 H     1 UNL1     0.1267
  12 O     4.0340  -3.3127 -13.7499 O.3   1 UNL1    -0.5991
  13 H     5.1176   0.4899 -15.2887 H     1 UNL1     0.1231
  14 H     3.5055   1.0447 -14.8385 H     1 UNL1     0.1322
  15 H     3.8185  -1.4454 -15.5677 H     1 UNL1     0.1331
  16 H     2.7437  -1.0877 -14.2046 H     1 UNL1     0.1675
  17 H     6.0025   0.5160 -13.1558 H     1 UNL1     0.1218
  18 H     2.5105  -2.5501 -12.0714 H     1 UNL1     0.1535
  19 H     3.7574  -3.2912 -11.0669 H     1 UNL1     0.1346
  20 H     1.9902  -2.1403  -9.6844 H     1 UNL1     0.1392
  21 H     3.5274  -1.2832  -9.4670 H     1 UNL1     0.1425
  22 H     2.4506   1.2994 -12.1713 H     1 UNL1     0.1492
  23 H     3.8353   2.7076 -13.1317 H     1 UNL1     0.1147
  24 H     0.0335  -0.6643 -10.5158 H     1 UNL1     0.1616
  25 H     0.7583   0.3210  -9.2519 H     1 UNL1     0.1612
  26 H     0.4278   1.0220 -10.8773 H     1 UNL1     0.1594
  27 H     6.6330  -1.2191 -13.9671 H     1 UNL1     0.1701
  28 H     6.5856  -2.9153 -13.4877 H     1 UNL1     0.1700
  29 H     6.1286  -2.4727 -15.1445 H     1 UNL1     0.1598
  30 H     5.4694   3.9178 -11.6501 H     1 UNL1     0.1480
  31 C     4.2714   0.0137 -12.0038 C.3   1 UNL1    -0.0600
  32 C     4.4630  -1.5405 -12.1454 C.3   1 UNL1    -0.1532
  33 C     4.6111  -1.9905 -13.6274 C.3   1 UNL1     0.4013
  34 C     3.7993  -1.0593 -14.5409 C.3   1 UNL1    -0.3665
  35 C     2.7509  -1.5317 -10.2124 C.3   1 UNL1    -0.3022
  36 C     3.3566  -2.3156 -11.3928 C.3   1 UNL1    -0.2400
  37 C     4.9192   0.8073 -13.1658 C.3   1 UNL1    -0.1306
  38 C     2.8482   0.4073 -11.7011 C.2   1 UNL1    -0.2653
  39 C     2.1444  -0.2699 -10.7893 C.2   1 UNL1     0.0852
  40 H     5.7231   4.1377 -13.9293 H     1 UNL1     0.1500
  41 H     6.7967   2.7249 -14.0435 H     1 UNL1     0.1488
  42 H     5.3962   2.8175 -15.1148 H     1 UNL1     0.1491
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  6    3   12   1
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  8   34   16   1
  9   34   33   1
 10    4   37   1
 11    9   41   1
 12    9   40   1
 13    9    5   1
 14    8   27   1
 15    8   33   1
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 23    5   10   1
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 27   32   36   1
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 29   31   38   1
 30   31    6   1
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 34   10    1   1
 35   36   19   1
 36   36   35   1
 37   26    7   1
 38   39    7   1
 39   39   35   1
 40   24    7   1
 41    7   25   1
 42   35   20   1
 43   35   21   1
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Compound 47

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compuesto_47.out
 42 44 0 0 0
SMALL
MULLIKEN_CHARGES

@<TRIPOS>ATOM
    1 H      1.6187  -1.1750 -14.1055 H      1 UNL1    0.1511
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    3 H      2.2146  -1.3627 -12.4086 H      1 UNL1    0.1602
    4 H      3.0349   3.5433 -14.5902 H      1 UNL1    0.1533
    5 H      1.8407   2.7535 -13.5718 H      1 UNL1    0.1502
    6 H      5.2688  -3.0630 -14.6192 H      1 UNL1    0.1563
    7 H      4.7569  -3.3038 -12.9006 H      1 UNL1    0.1857
    8 H      3.7249  -3.7414 -14.2238 H      1 UNL1    0.1372
    9 C      4.0607   0.0050 -11.6938 C.3    1 UNL1   -0.3569
   10 C      4.5547   1.4143 -14.2194 C.3    1 UNL1   -0.1141
   11 C      3.4712   0.6653 -15.0287 C.3    1 UNL1   -0.2984
   12 C      5.5786   0.3715 -13.6867 C.3    1 UNL1    0.0772
   13 C      4.7356  -0.6948 -12.8881 C.3    1 UNL1    0.2902
   14 C      6.2912  -0.3609 -14.8541 C.3    1 UNL1   -0.2970
   15 C      3.8246  -1.5598 -13.8612 C.3    1 UNL1    0.1658
   16 C      3.8596  -0.8148 -15.2405 C.3    1 UNL1   -0.1079
   17 C      5.2610  -0.8672 -15.8665 C.3    1 UNL1   -0.2696
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18 C	3.2230	1.2339	-12.0419	C.3	1	UNL1	-0.2645
19 C	3.8999	2.1921	-13.0531	C.3	1	UNL1	-0.0458
20 O	5.6562	-1.6544	-12.3031	O.3	1	UNL1	-0.5992
21 C	6.6816	1.0394	-12.8407	C.3	1	UNL1	-0.5214
22 C	2.8576	3.2044	-13.5563	C.3	1	UNL1	-0.4970
23 C	4.4237	-2.9762	-13.9220	C.3	1	UNL1	-0.5080
24 C	2.3455	-1.7109	-13.4428	C.3	1	UNL1	-0.5222
25 H	5.4873	-1.9081	-16.1777	H	1	UNL1	0.1300
26 H	5.3061	-0.2495	-16.7785	H	1	UNL1	0.1273
27 H	3.1320	-1.2959	-15.9273	H	1	UNL1	0.1186
28 H	7.0185	0.2849	-15.3728	H	1	UNL1	0.1280
29 H	6.8731	-1.2153	-14.4249	H	1	UNL1	0.1485
30 H	3.2571	1.1444	-16.0071	H	1	UNL1	0.1267
31 H	2.5190	0.7137	-14.4684	H	1	UNL1	0.1422
32 H	5.0910	2.1490	-14.8617	H	1	UNL1	0.1227
33 H	4.8638	0.2887	-10.9991	H	1	UNL1	0.1374
34 H	3.4708	-0.7282	-11.0993	H	1	UNL1	0.1501
35 H	2.2451	0.9141	-12.4577	H	1	UNL1	0.1370
36 H	3.0218	1.7964	-11.1088	H	1	UNL1	0.1255
37 H	4.7038	2.7518	-12.5177	H	1	UNL1	0.1152
38 H	6.3352	-1.2194	-11.7715	H	1	UNL1	0.3030
39 H	7.4469	0.2892	-12.6272	H	1	UNL1	0.1493
40 H	7.1468	1.8544	-13.4112	H	1	UNL1	0.1575
41 H	6.3850	1.4965	-11.8822	H	1	UNL1	0.1556
42 H	2.8376	4.0703	-12.8722	H	1	UNL1	0.1471

@<TRIPOS>BOND
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 9   16   15   1
10   11   31   1
11   11   10   1
12   32   10   1
13   14   29   1
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16    4   22   1
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19   10   19   1
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23   15   24   1
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25   12   13   1
26   12   21   1
27    5   22   1
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34   19   18   1
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37   21   39   1
38   21   41   1
39   35   18   1
40   20   38   1
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43   9  34  1
44   9  33  1
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