

Supporting information 2

On Benchmarking of Automated Methods for Performing Exhaustive Reaction Path Search

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Table SI2: An input file for SC-AFIR1 search.

```
-----
# SC-AFIR/B3LYP/6-31+G* IOp(5/5=3)

0 1
C      4.412142554513      0.122166522737      0.267819299889
C      2.900728682935      0.194730725884      0.238311426237
C      2.283358940631     -0.632233661209      1.370215518551
H      4.841947786326     -0.902885109191      0.217925964279
H      2.585510669119      1.240759947656      0.287271639807
H      2.563913079071     -0.230502676930     -0.719353858055
H      2.457722011146     -0.165290844045      2.348345270979
H      2.687368526866     -1.653375120562      1.386789858303
O      0.885396456960     -0.683675863088      1.095502431559
O      0.294561222952     -1.522161102174      2.132217173858
H     -0.350591951268     -0.898057650651      2.512076908730
O      5.144259020750      1.086234831573      0.332164365866

Options
GauMem=800
GauProc=4
NoBondRearrange
Add Interaction
Gamma=1000
END
NOFC
-----
```

Table SI3: An input file for SC-AFIR2 search.

```
-----
# SC-AFIR2/B3LYP/6-31+G* IOp(5/5=3)

0 1
C      4.412142554513      0.122166522737      0.267819299889
C      2.900728682935      0.194730725884      0.238311426237
C      2.283358940631     -0.632233661209      1.370215518551
H      4.841947786326     -0.902885109191      0.217925964279
H      2.585510669119      1.240759947656      0.287271639807
H      2.563913079071     -0.230502676930     -0.719353858055
H      2.457722011146     -0.165290844045      2.348345270979
H      2.687368526866     -1.653375120562      1.386789858303
O      0.885396456960     -0.683675863088      1.095502431559
O      0.294561222952     -1.522161102174      2.132217173858
H     -0.350591951268     -0.898057650651      2.512076908730
O      5.144259020750      1.086234831573      0.332164365866

Options
GauMem=800
GauProc=4
NoBondRearrange
Add Interaction
Gamma=1000
END
NOFC
-----
```

Table SI4: An input file for SC-AFIR1+ initial search with a weak artificial force of $\gamma =$

10 / ($N - 1$) kJ/mol added between all pairs of atoms.

SC-AFIR/B3LYP/6-31+G* IOp(5/5=3)

0 1

C	4.187607658197	0.053851031706	0.482538005806
C	2.796342769937	0.180246477660	0.027151147802
C	2.196776549552	-0.584695670974	1.145884791682
H	4.637444952278	-0.908111160549	0.218217906213
H	2.427940819740	1.188699360086	0.058420892741
H	2.592054487181	-0.341314652683	-0.891338703932
H	2.382326479126	-0.008890608408	2.052359803926
H	2.665158341458	-1.555747410611	1.260270756002
O	0.837740088086	-0.718664799256	0.923148936815
O	0.417752198148	-1.364985061532	2.135281015508
H	0.886290349043	-0.786391994443	2.764733319721
O	4.678882307244	0.801714489008	1.292618127712

Options

GauMem=800

GauProc=8

NoBondRearrange

Add Interaction

Gamma=1000.0

Fragm.1=1

Fragm.2=2

Fragm.3=3

Fragm.4=4

Fragm.5=5

Fragm.6=6

Fragm.7=7

Fragm.8=8

Fragm.9=9

Fragm.10=10

Fragm.11=11

Fragm.12=12

1	2	0.909090909
1	3	0.909090909
1	4	0.909090909
1	5	0.909090909
1	6	0.909090909
1	7	0.909090909
1	8	0.909090909
1	9	0.909090909
1	10	0.909090909
1	11	0.909090909
1	12	0.909090909

2	3	0.909090909
2	4	0.909090909
2	5	0.909090909
2	6	0.909090909
2	7	0.909090909
2	8	0.909090909
2	9	0.909090909
2	10	0.909090909
2	11	0.909090909
2	12	0.909090909
3	4	0.909090909
3	5	0.909090909
3	6	0.909090909
3	7	0.909090909
3	8	0.909090909
3	9	0.909090909
3	10	0.909090909
3	11	0.909090909
3	12	0.909090909
4	5	0.909090909
4	6	0.909090909
4	7	0.909090909
4	8	0.909090909
4	9	0.909090909
4	10	0.909090909
4	11	0.909090909
4	12	0.909090909
5	6	0.909090909
5	7	0.909090909
5	8	0.909090909
5	9	0.909090909
5	10	0.909090909
5	11	0.909090909
5	12	0.909090909
6	7	0.909090909
6	8	0.909090909
6	9	0.909090909
6	10	0.909090909
6	11	0.909090909
6	12	0.909090909
7	8	0.909090909
7	9	0.909090909
7	10	0.909090909
7	11	0.909090909
7	12	0.909090909
8	9	0.909090909
8	10	0.909090909
8	11	0.909090909
8	12	0.909090909
9	10	0.909090909

9	11	0.909090909
9	12	0.909090909
10	11	0.909090909
10	12	0.909090909
11	12	0.909090909

END

NOFC

EQOnly

KeepLUPPath

Table SI5: An input file for a refinement of the paths obtained by the SC-AFIR1+ search

shown in **Table SI4**.

```
-----
%infile=test_SC0a
# RePATH/B3LYP/6-31+G* IOp(5/5=3)

0 1
C      4.335352298403      0.114591208596      0.335458577558
C      2.852191524106      0.178749642368      0.153606394523
C      2.258966911658     -0.639239939525      1.281760405748
H      4.780589870031     -0.875156977850      0.115332749840
H      2.500860529756      1.207085203944      0.200621036200
H      2.564307016250     -0.282891274702     -0.793527274118
H      2.444188461148     -0.145254811007      2.240885405466
H      2.682517519657     -1.646496656444      1.313894693444
O      0.871414179171     -0.711469505329      1.022646305647
O      0.314598215145     -1.489420768511      2.104428772969
H      0.090402828449     -0.777091104377      2.729003214488
O      5.010927646218      1.022304982846      0.765175718224

Options
GauMem=800
GauProc=8
NoBondRearrange
NOFC
-----
```