Table S1. Quantum mechanics B3LYP calculated total energies (hartree) and relative energies (kJ/mol) for fluorinated alkanes.

B3LYP//6-311+G**	Total Energy (hartree)	Relative Energy (kJ/mol)
1,1-difluoroethane	-278.416924	0
1,2-difluoroethane	-278.396916	53
1,1-difluoropropane	-317.743564	0
1,2-difluoropropane	-317.731709	31
1,1-difluorohexane	-435.700378	0
1,2-difluorohexane	-435.689045	30
2,2-difluorohexane	-435.709362	-24
3,3-difluorohexane	-435.708695	-22
2,4-difluorohexane	-435.701172	-2
2,5-difluorohexane	-435.701172	-2
1,1-difluorooctane	-514.34905	0
1,2-difluorooctane	-514.337696	30
3,6-difluorooctane	-514.349403	-3
2,6-difluorooctane	-514.348424	0
3,3-difluorooctane	-514.35745	-21
1,8-difluorooctane	-514.33608	32
2,7-difluorooctane	-514.349478	-3
2,3-difluorooctane	-514.344901	9
1,1-difluorononane	-553.673394	0
1,2-difluorononane	-553.662032	30
2,2-difluorononane	-553.682369	-24
3,3-difluorononane	-553.681789	-22
2,2,7,7 tetrafluorooctane	-712.913327	0
4,4,5,5 tetrafluorooctane	-712.899682	36
2,2,8,8-tetrafluorononane	-752.237282	0
4,4,5,5 tetrafluorononane	-752.22417	34
1,1,9,9 tetrafluorononane	-752.218726	49
1,1,2,2 tetrafluorononane	-752.214191	61
2,4,6,8 tetrafluorononane	-752.218128	50