

Chemistry–A European Journal

Supporting Information

YfeX – A New Platform for Carbene Transferase Development with High Intrinsic Reactivity

Victor Sosa Alfaro, Sodiq O. Waheed, Hannah Palomino, Anja Knorrscheidt,
Martin Weissenborn, Christo Z. Christov,* and Nicolai Lehnert*

Table of Contents	Page
Stability of WT YfeX carbene intermediate	S4
Scheme for metalation and CO removal of RuMPIX	S4
UV-vis spectra of metalated RuMPIX	S5
Reduction of reconstituted RuYfeX	S6
Stability test of the RuYfeX carbene intermediate	S7
Reduction of reconstituted CoYfeX	S7
Reduction of CoYfeX and stability of CoYfeX carbene intermediate	S7
Circular dichroism spectra of wild-type YfeX	S8
Circular dichroism spectra of YfeX at various methanol percentages	S9
UV-visible spectra of YfeX at various methanol percentages	S10
Carbene transfer reactivity of WT YfeX in the presence of methanol	S10
Carbene transfer reactivity of WT YfeX in the presence of DMSO	S11
Circular dichroism spectra of YfeX R232A at various methanol percentages	S13
N-H Insertion Products- GC/MS chromatogram data	S14- S28
Cyclopropanation Products- GC/MS chromatogram data	S29- S33
Si-H Insertion Products- GC/MS chromatogram data	S34
GC/MS chromatogram data for RuYfeX	S35-S40

GC/MS chromatogram data for RuYfeX	S41-S42
GC/MS chromatogram data for CoYfeX	S43-S45
20 mg scale-up reactivity for N-H insertion via YfeX	S46
YfeX substrate ratio optimization for N-H insertion reactivity	S47
Supercritical fluid chromatography of styrene cyclopropanation	S48-S51
Supercritical fluid chromatography of co-solvent reactivity	S52-S54
Calibration Curves for standard products	S55-S58
Dynamics of the hydrophobic interactions	S59
Dynamics of the π - π stacking and cation- π stacking interactions	S59
Stationary point geometries involved in the Si-H insertion reaction in YfeX	S60
The Cartesian coordinates of the optimized QM regions of the QM/MM geometries	S61-S67

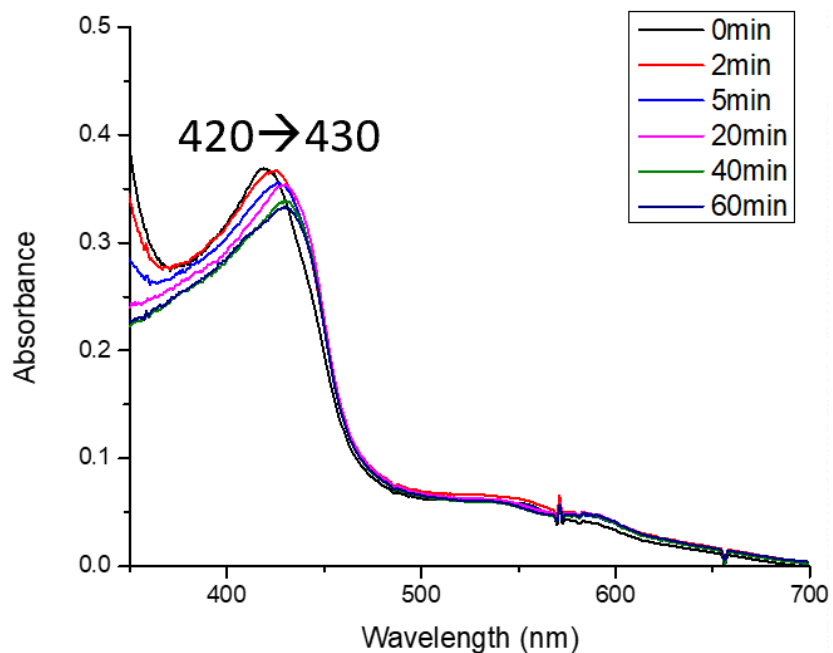


Figure S1. Stability of the wild type (WT) YfeX [10 μ M] carbene intermediate under catalytic conditions after the addition of dithionite [20 mM] and EDA [10 mM], followed by UV-vis spectroscopy in [100 mM] potassium phosphate buffer.

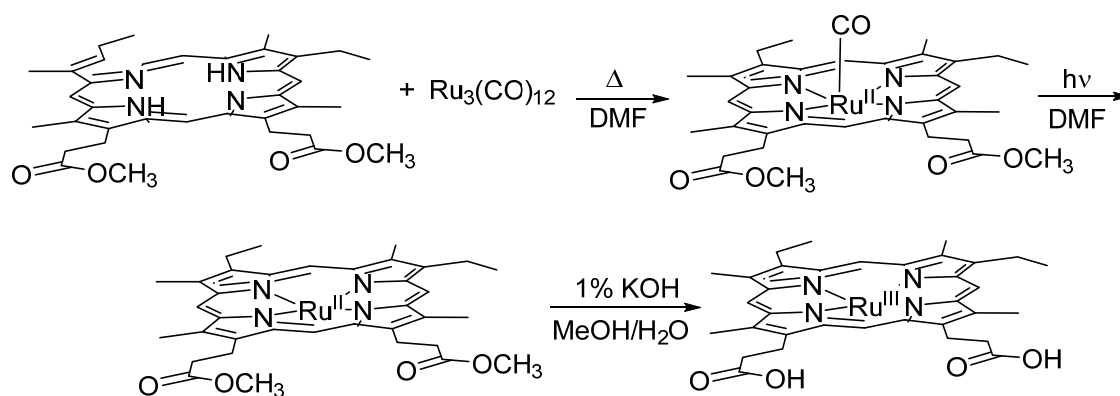


Figure S2. Scheme for the metalation of H₂[MpIX] and the following CO removal and ester hydrolysis to yield [RuMpIX]⁺.

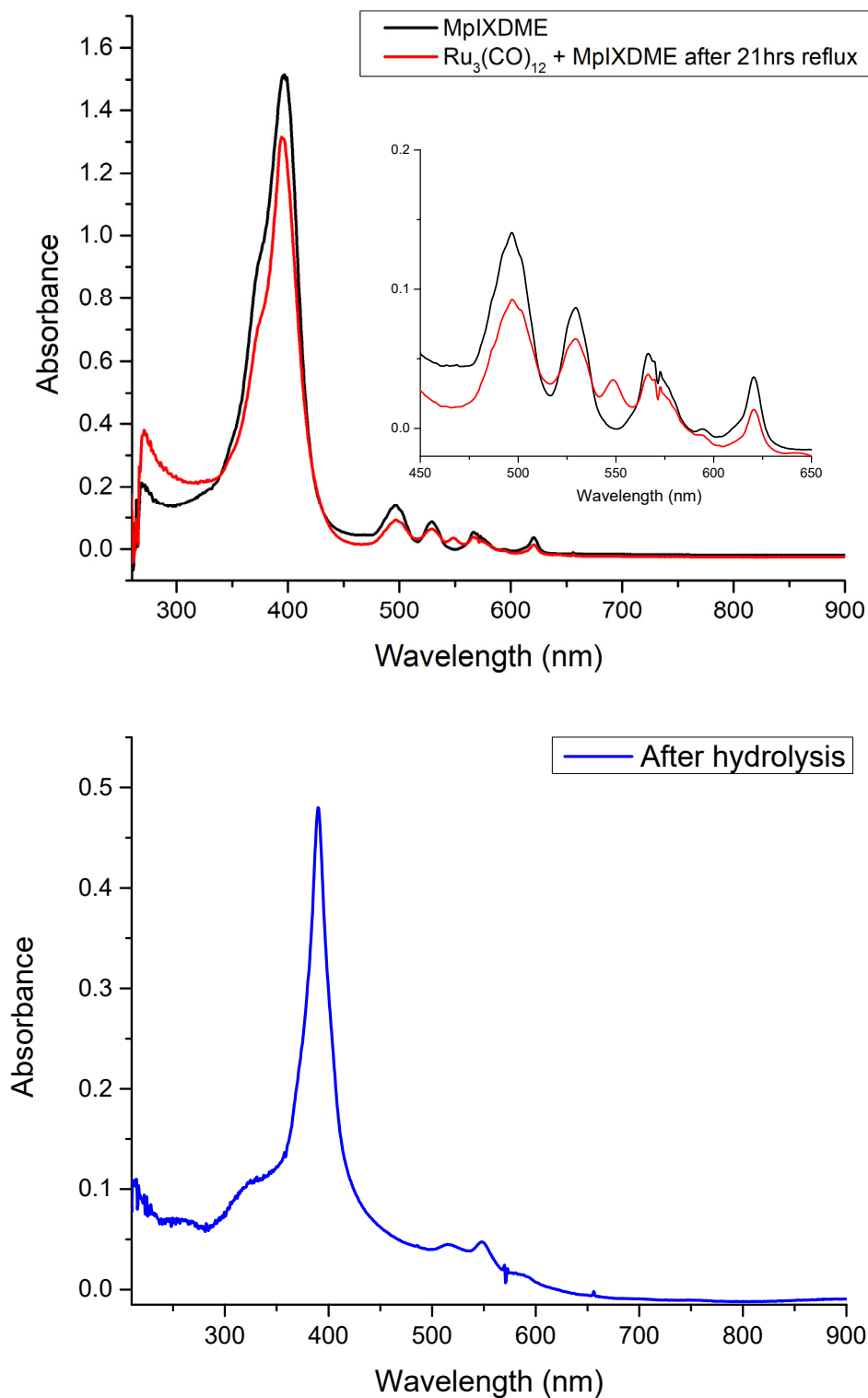


Figure S3. UV-vis spectra of (a) metalated H₂[MplX] with Ru₃(CO)₁₂ and (b) [RuMplX]⁺ after photolysis and ester hydrolysis.

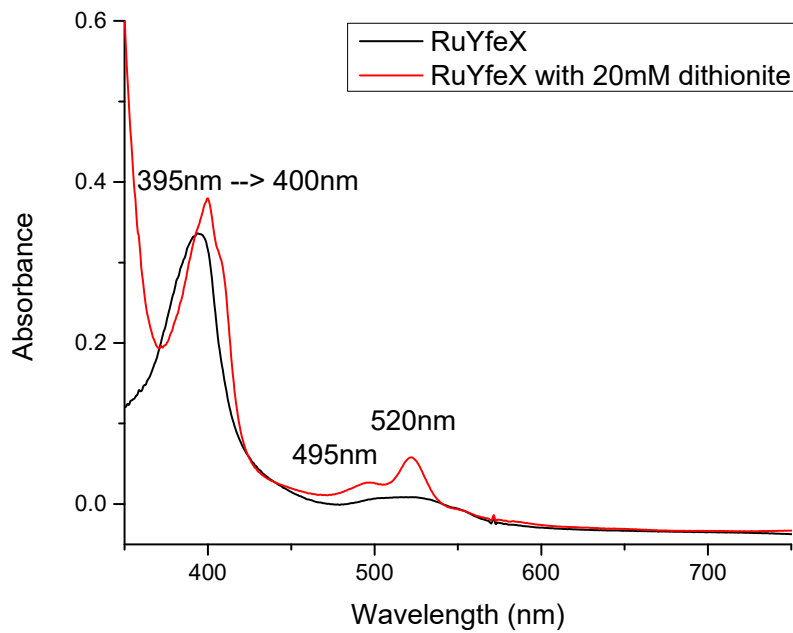
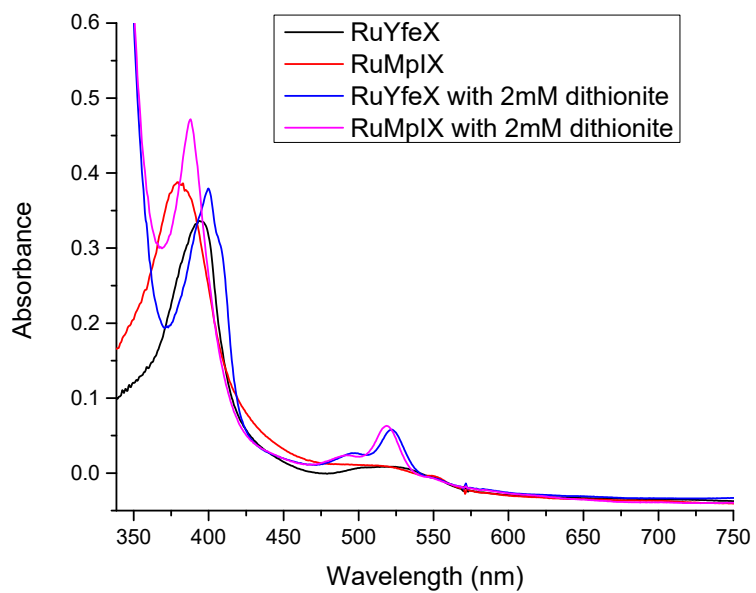


Figure S4. Reduction of RuYfeX, which corresponds to apo-YfeX reconstituted with Ruthenium-mesoporphyrin IX, followed by UV-vis spectroscopy.

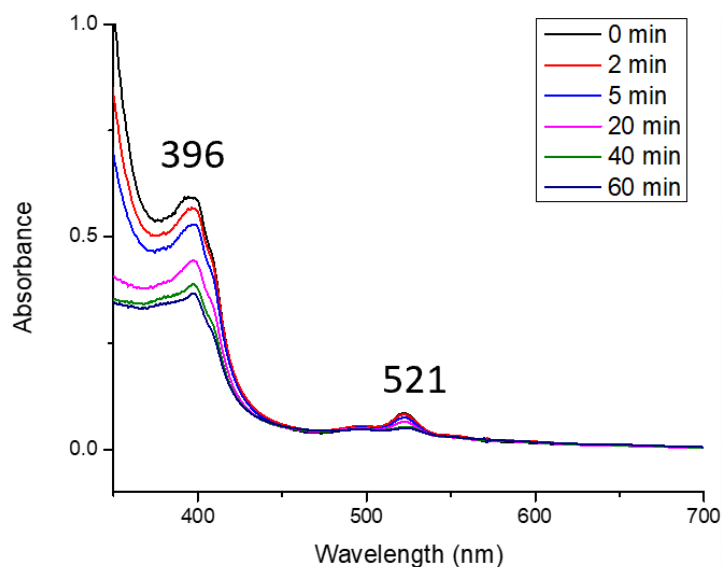


Figure S5. Stability of the carbene intermediate of RuYfeX [20 μM] under catalytic conditions, generated by addition of EDA [20 mM] to Ru(II)YfeX, followed by UV-vis spectroscopy in pH 7.4 [100 mM] potassium phosphate buffer.

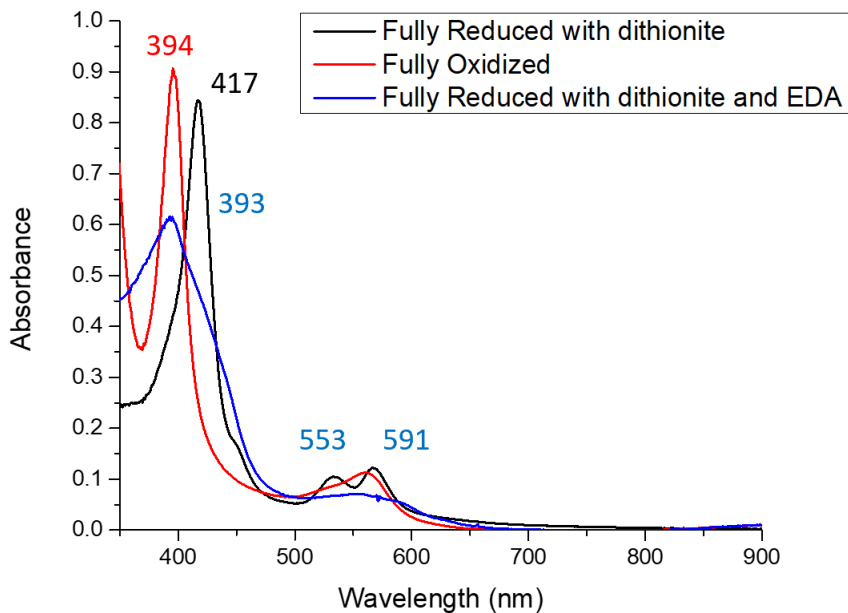


Figure S6. UV-vis spectra of CoYfeX [10 μM], which corresponds to apo-YfeX reconstituted with Cobalt-protoporphyrin IX, in the oxidized form (red line), after reduction with sodium dithionite [20 mM] (black line), and after generation of the carbene intermediate via addition of dithionite [20 mM] and EDA [10 mM] (blue line).

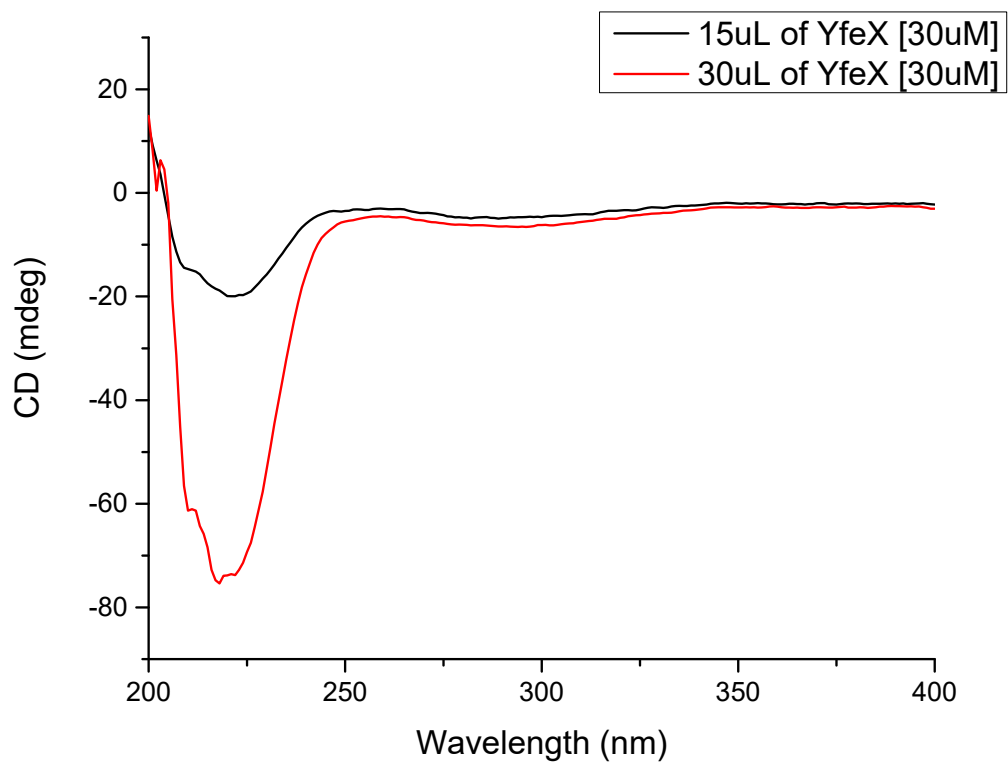


Figure S7. Circular dichroism spectra of WT YfeX at pH 7.4 in [100 mM] potassium phosphate buffer.

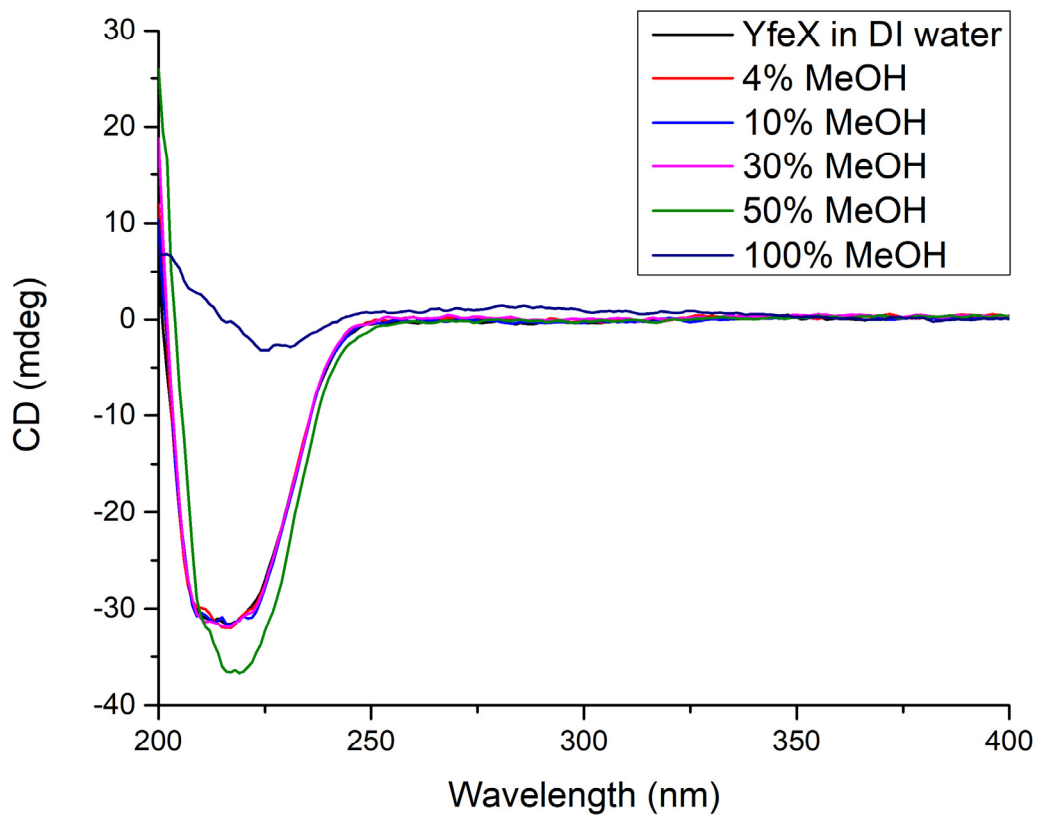


Figure S8. Circular dichroism spectra of WT YfeX [30µM] at various buffer/methanol mixtures. The data show that at 50% methanol concentration structural changes to the protein occur.

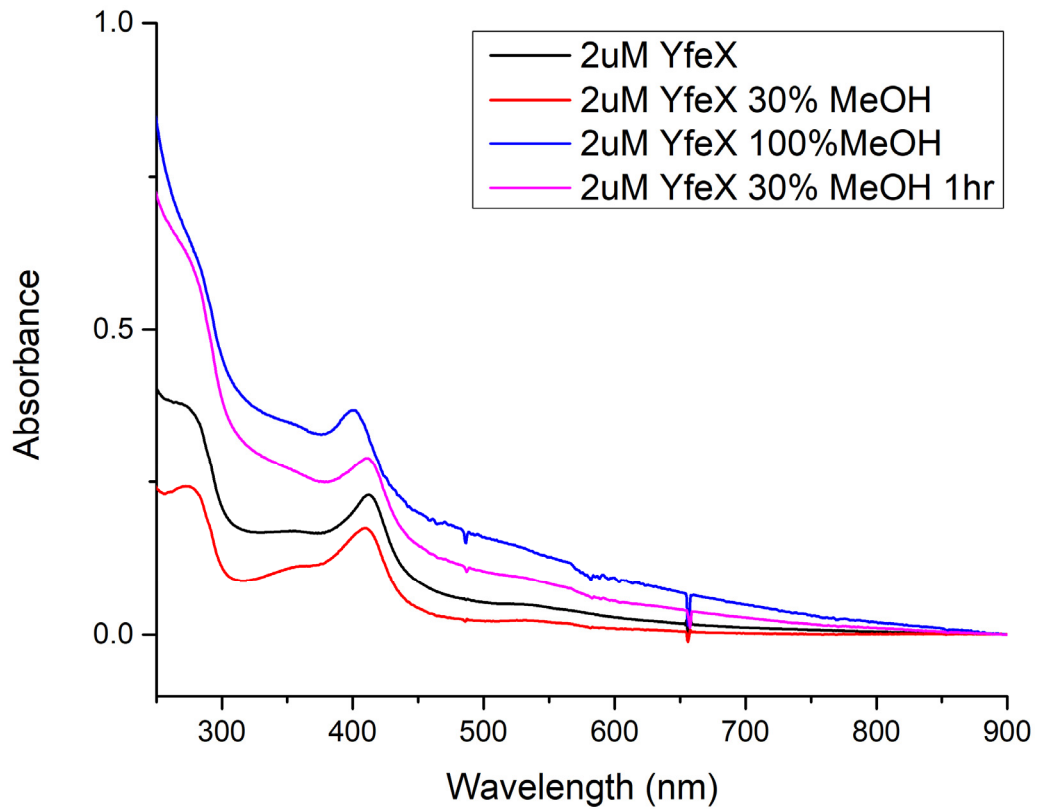
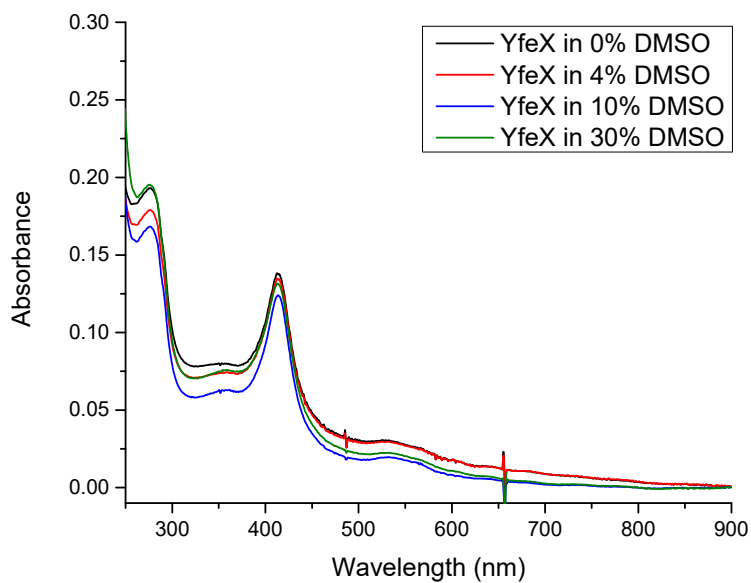


Figure S9. UV-visible spectra of WT YfeX [30 μ M] at various buffer/methanol mixtures. The data show that WT YfeX is stable in 30% MeOH (red spectrum), but that after 1 hour some precipitation occurs (purple spectrum), indicated by the rise in scattering background. However, in 100% MeOH the protein degrades and precipitates, and heme is released (blue spectrum).

(A)



(B)

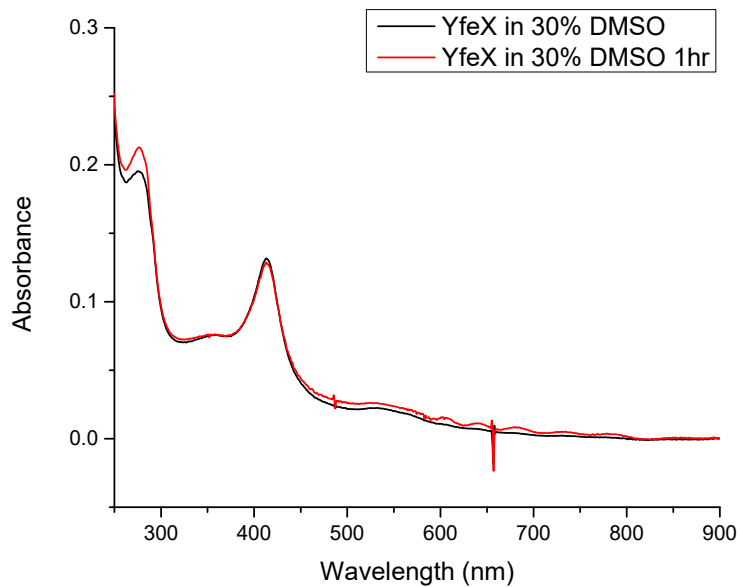


Figure S10. UV-visible spectra of (A) WT YfeX [30 μM] in various buffer/DMSO mixtures. The data show that WT YfeX is stable in 30% DMSO (blue spectrum). (B) UV-visible spectra of YfeX in 30% DMSO before and after 1 hour.

Table S1. Carbene transfer reactivity of WT YfeX in the presence of methanol and DMSO co-solvent.

[% Methanol]	Aniline (% yield)	Styrene (% yield)	Cis:Trans	Trans (R,R)
0	72 ± 32	27 ± 7.2	11:89	87%
10	50.9 ± 4.3	-----		
30	51.0 ± 3.8	47.4 ± 1.5	9:91	87%
50	40.2 ± 2.6	39.2 ± 2.9		

[% DMSO]	Aniline (% yield)	Styrene (% yield)	Cis:Trans	Trans (R,R)
30	71 ± 51	59 ± 8.1	9:91	88%

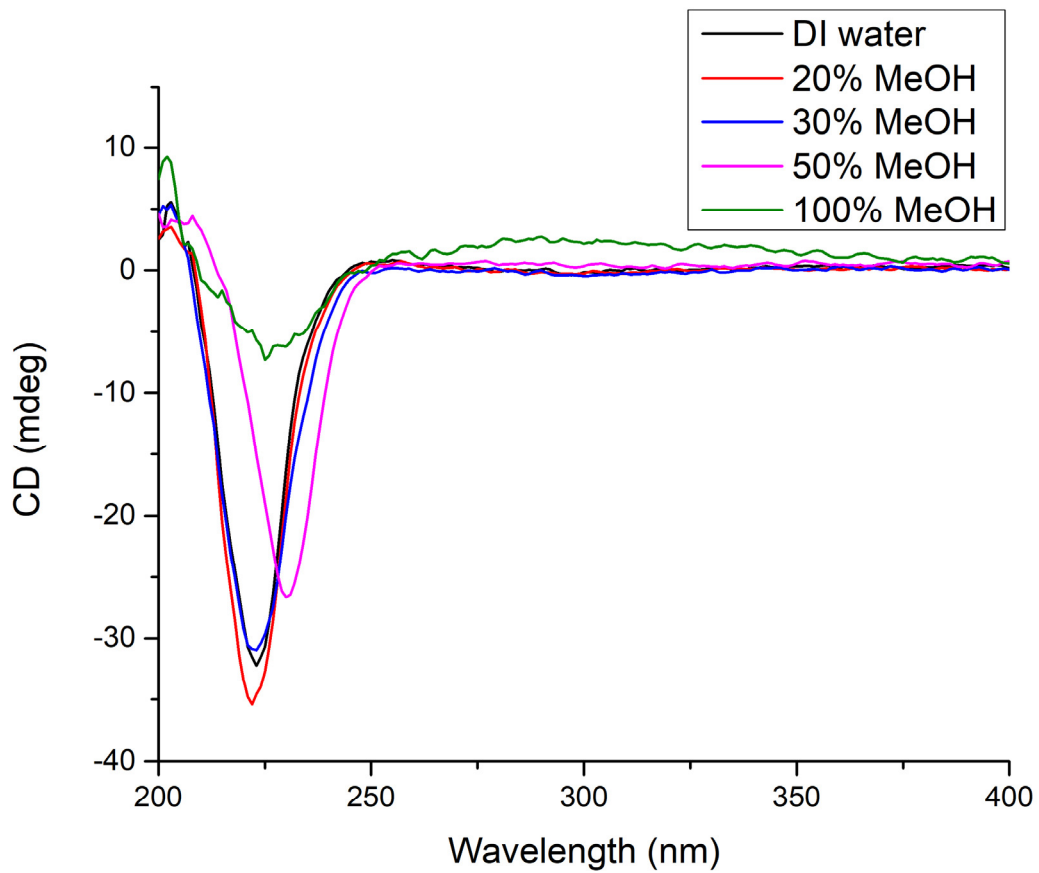
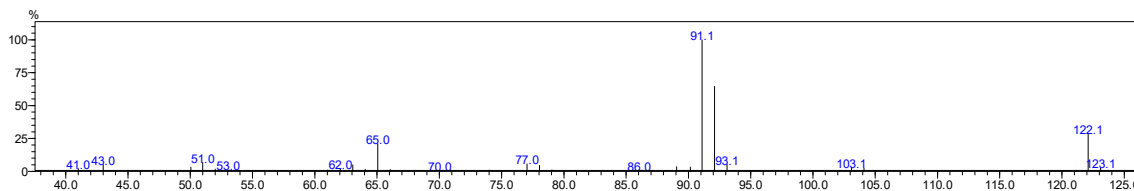
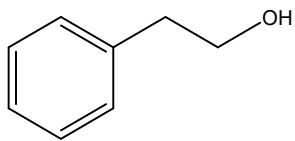
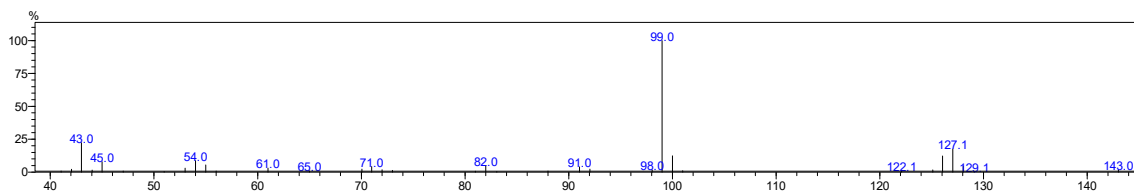
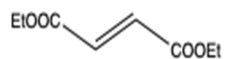


Figure S11. Circular dichroism spectra of YfeX R232A [20µM] at various buffer/methanol mixtures.

N-H Insertion Products- GC/MS chromatogram data

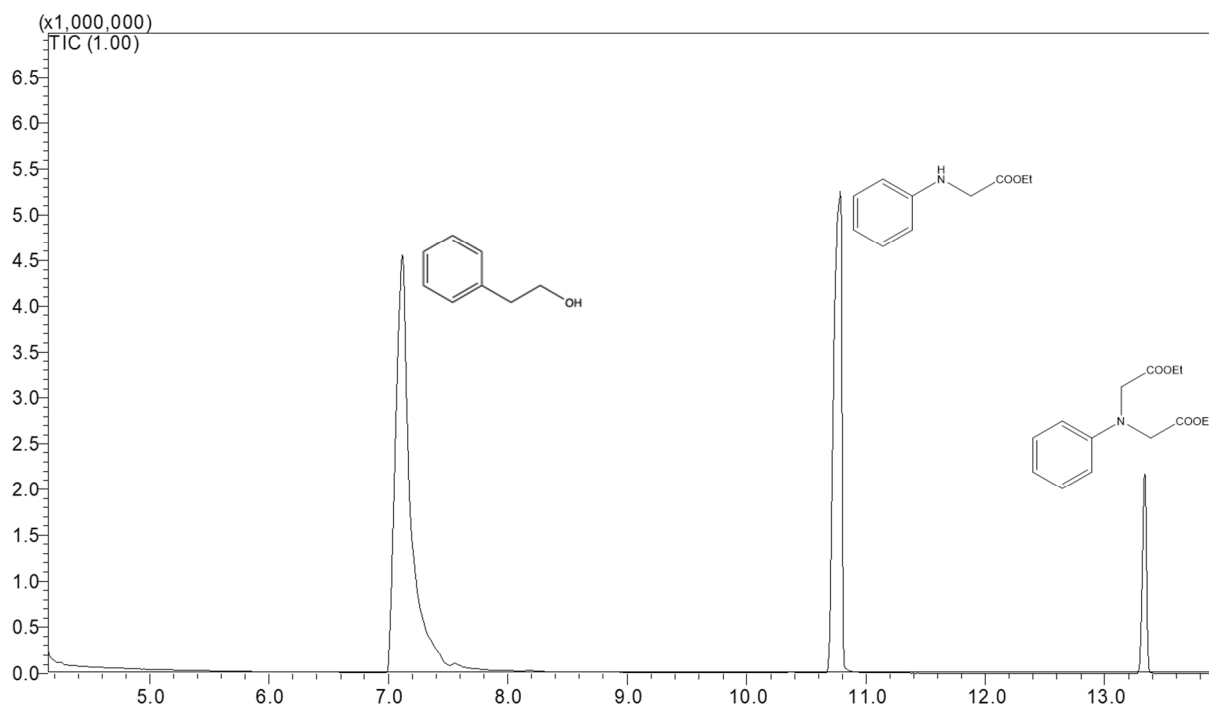


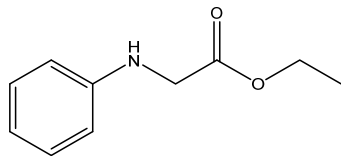
Internal standard: 2-phenyl ethanol.



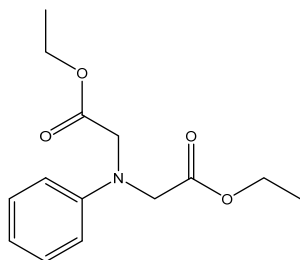
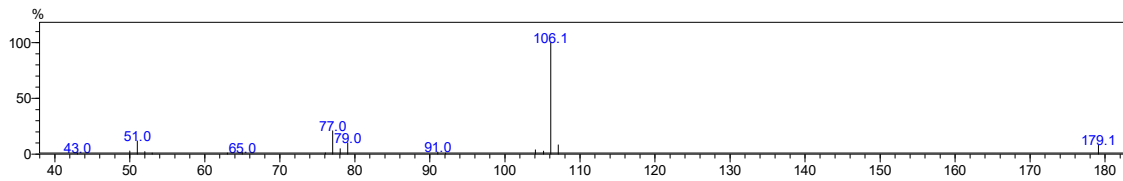
Diethyl 2-butenedioate from ethyl diazo acetate (EDA) dimer product.

YfeX 0.1mol Aniline

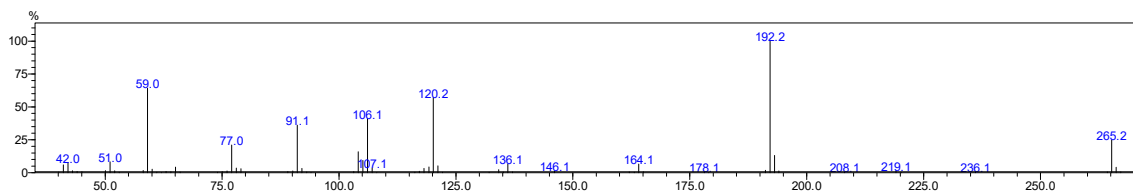




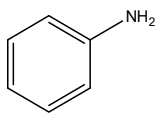
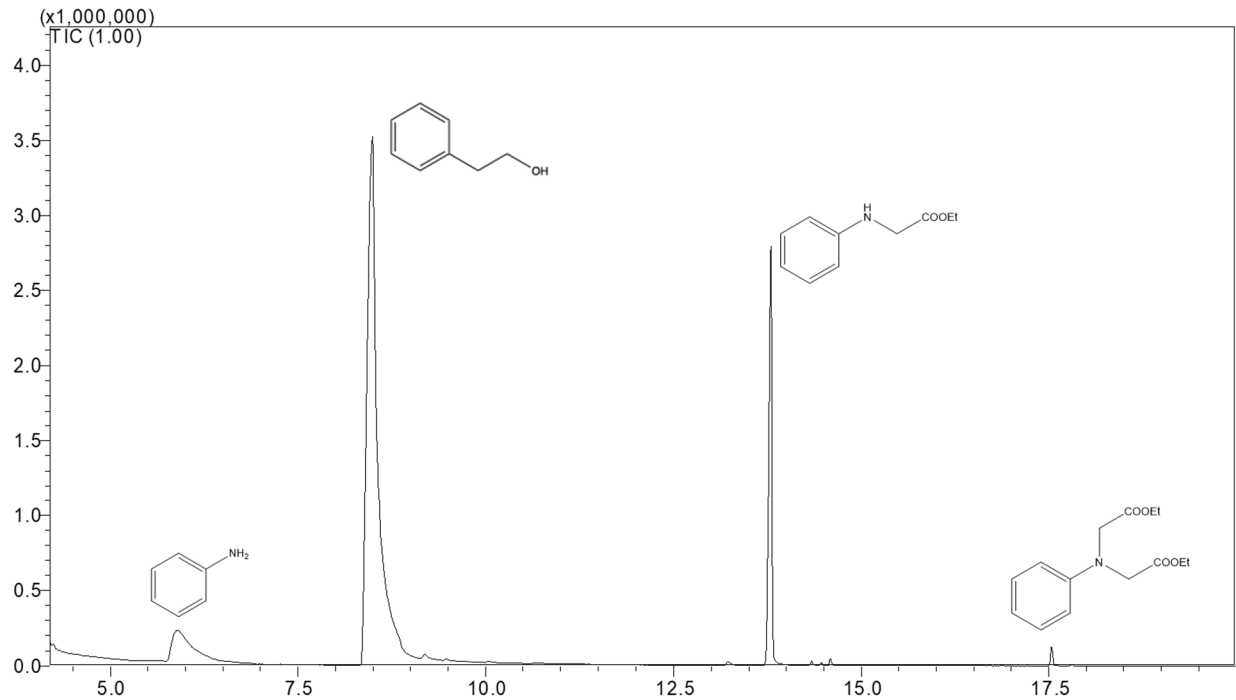
Molecular Weight: 179.22



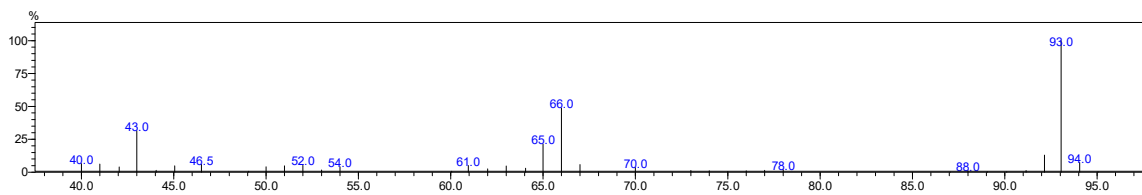
Molecular Weight: 265.31



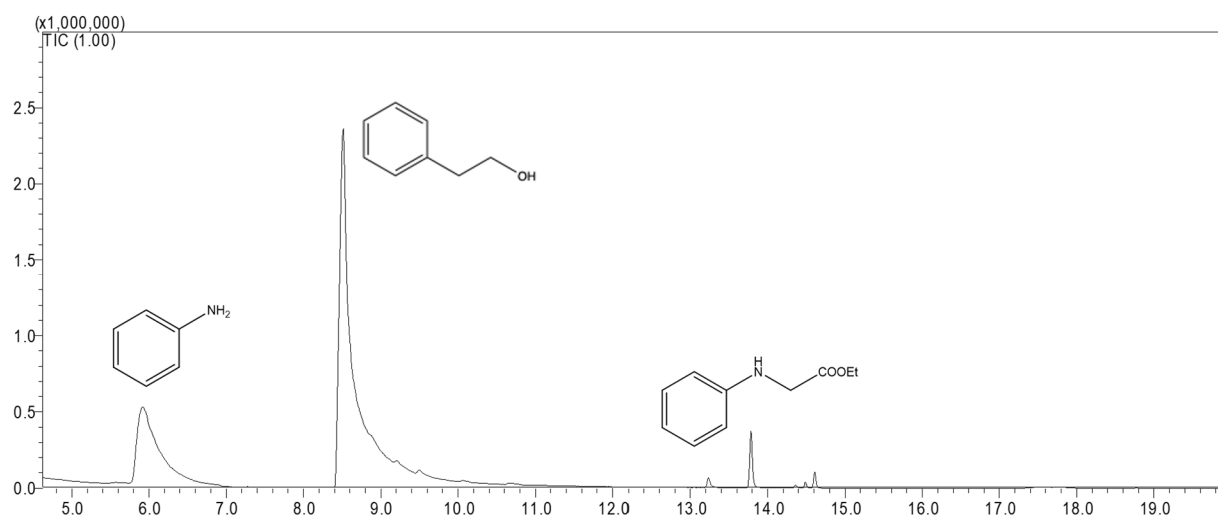
YfeX 0.01mol Aniline



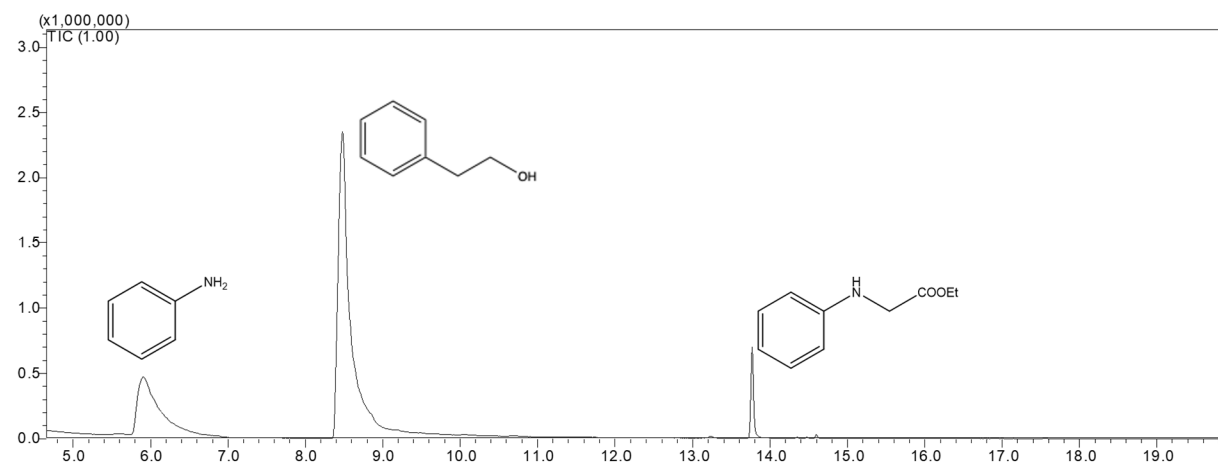
Molecular Weight: 93.13



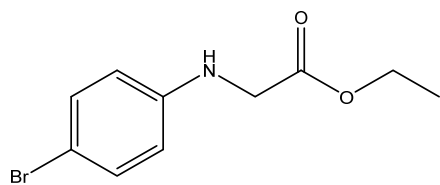
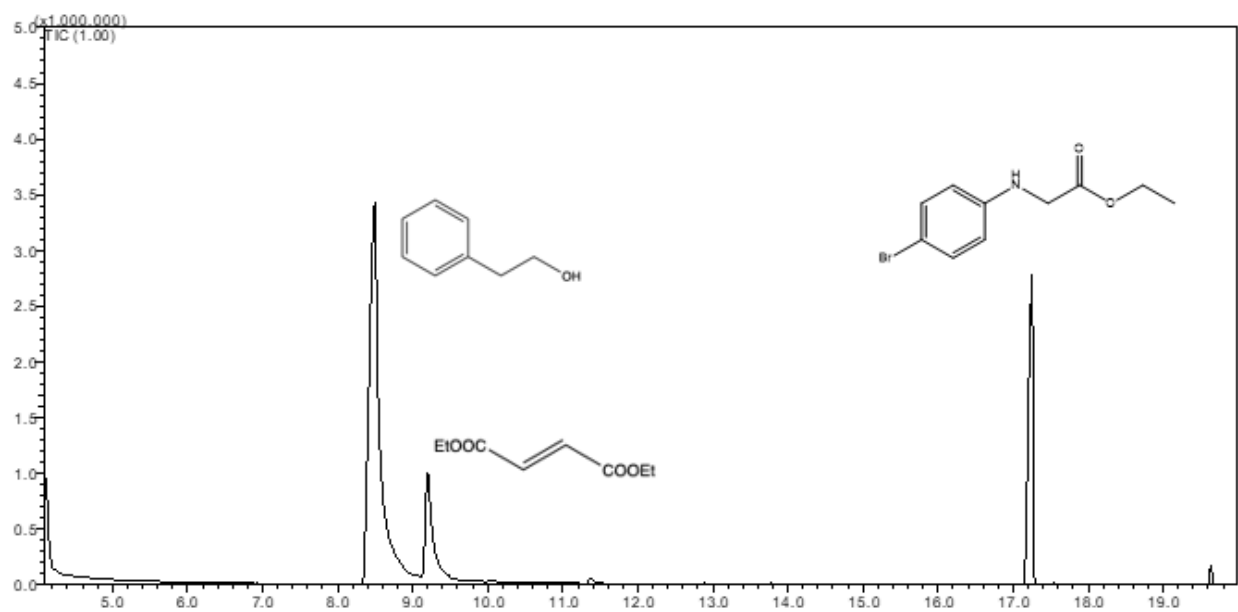
YfeX 0.001mol Aniline



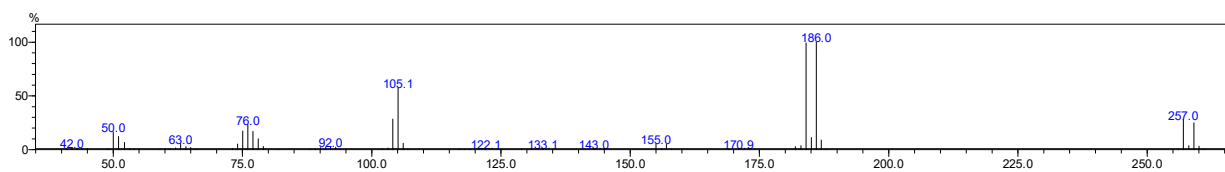
YfeX 0.001mol Aniline 20hrs



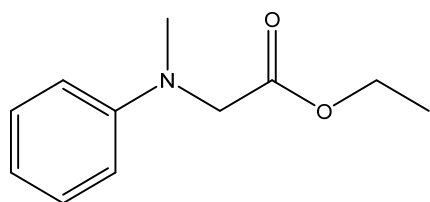
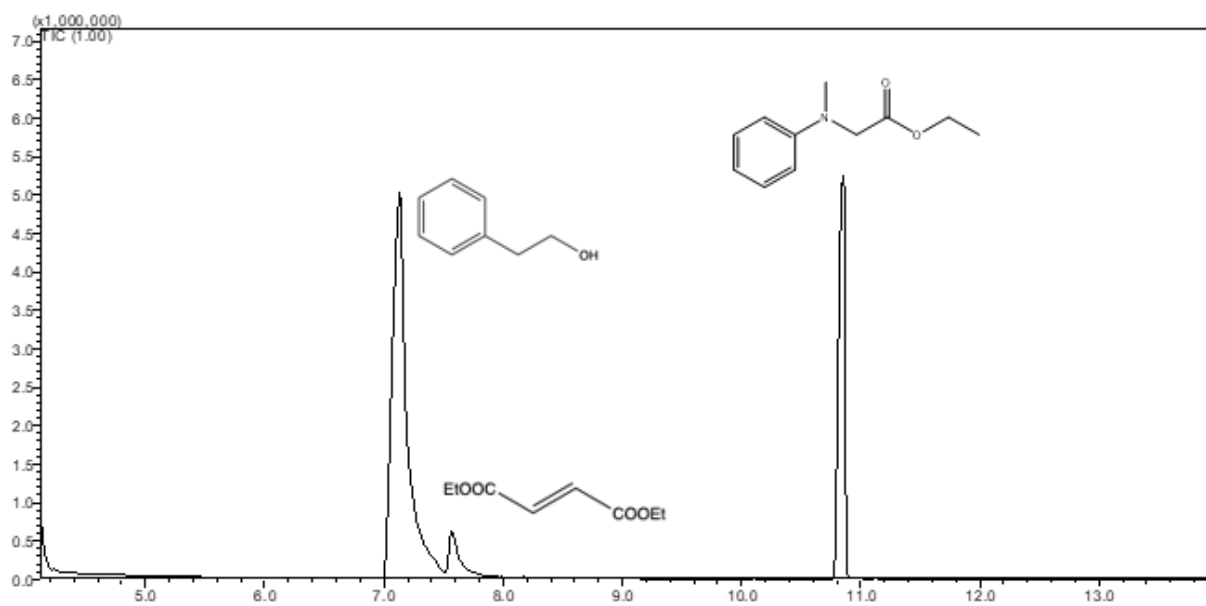
4-Bromoaniline



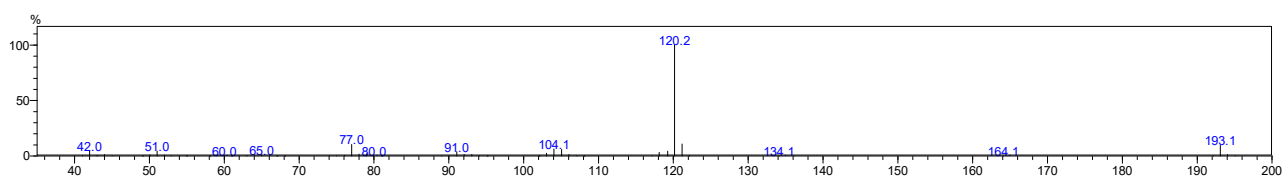
Molecular Weight: 258.12



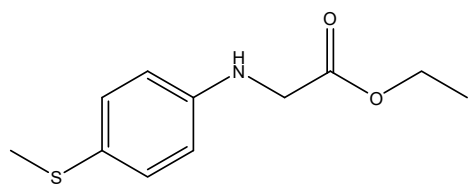
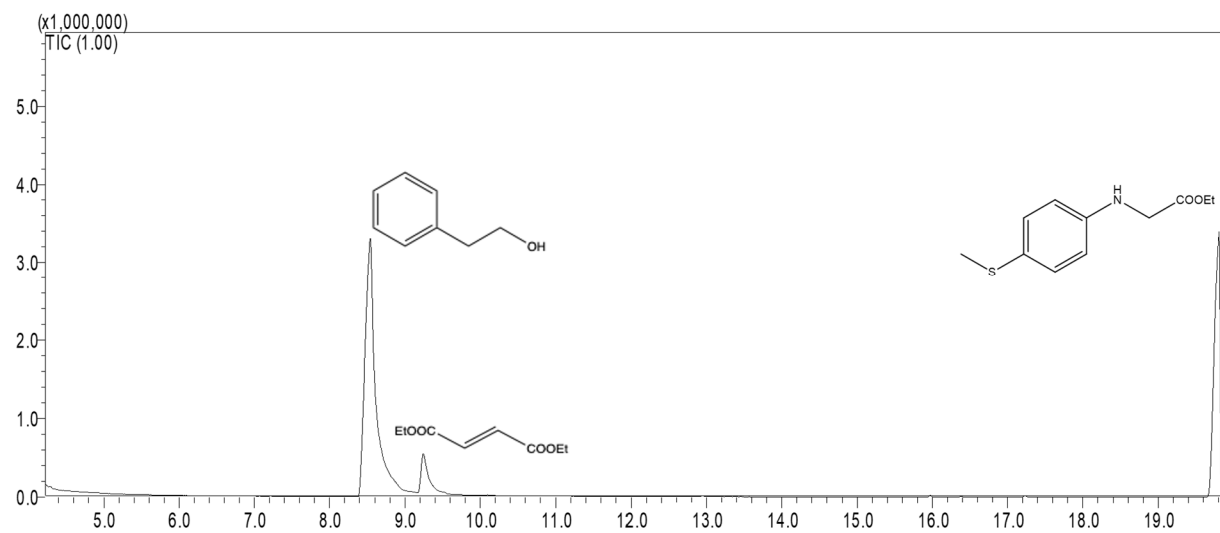
N-methylaniline



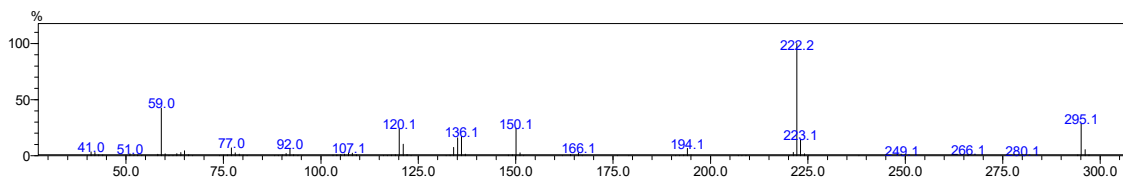
Molecular Weight: 193.25



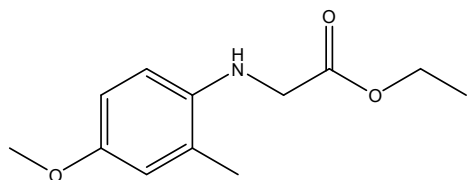
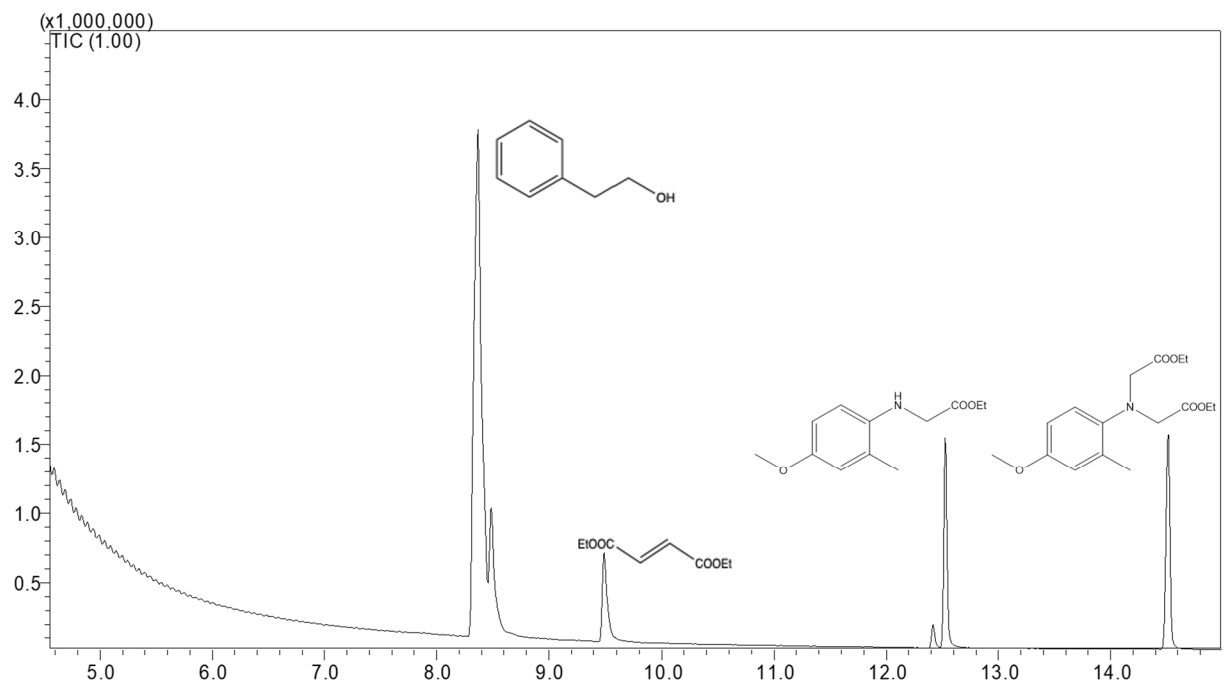
4-Methylthiolaniline



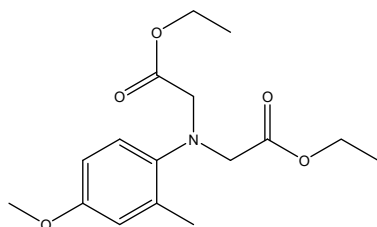
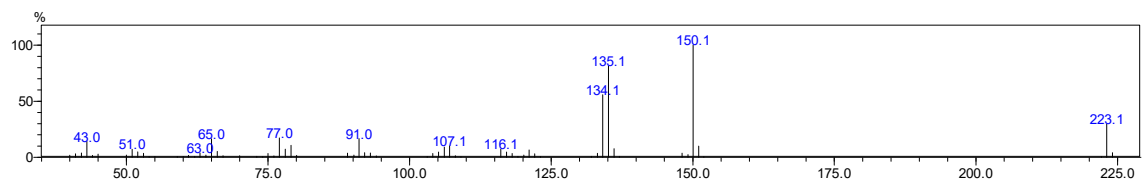
Molecular Weight: 225.31



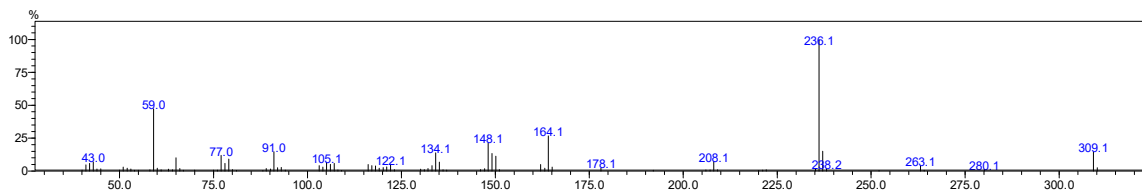
6-Methyl-4-methoxyaniline



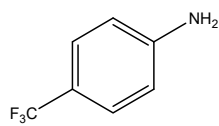
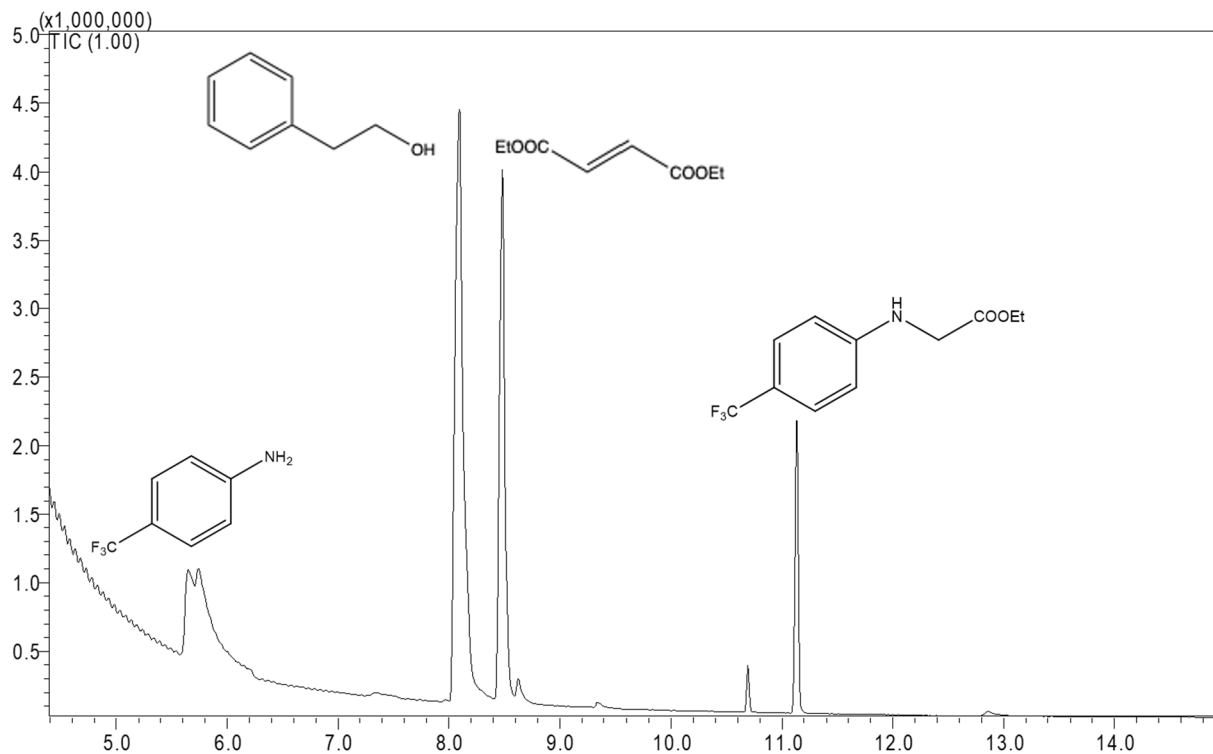
Molecular Weight: 223.27



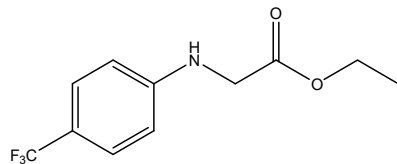
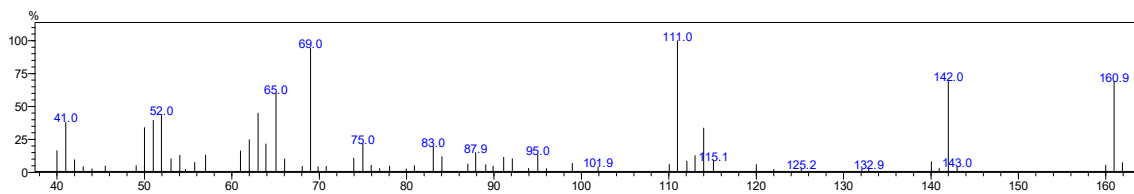
Molecular Weight: 309.36



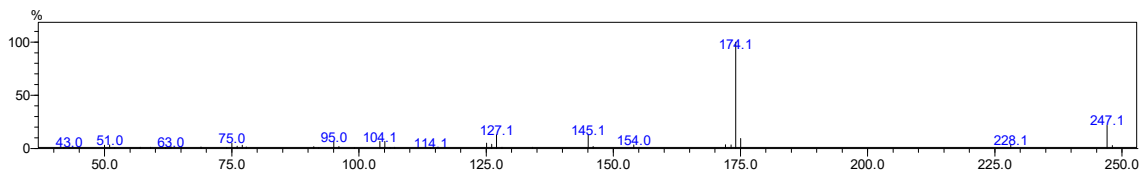
4-Trifluoromethylaniline



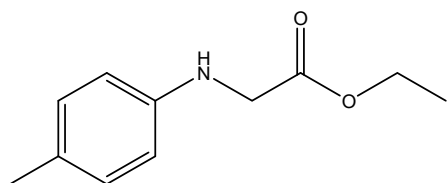
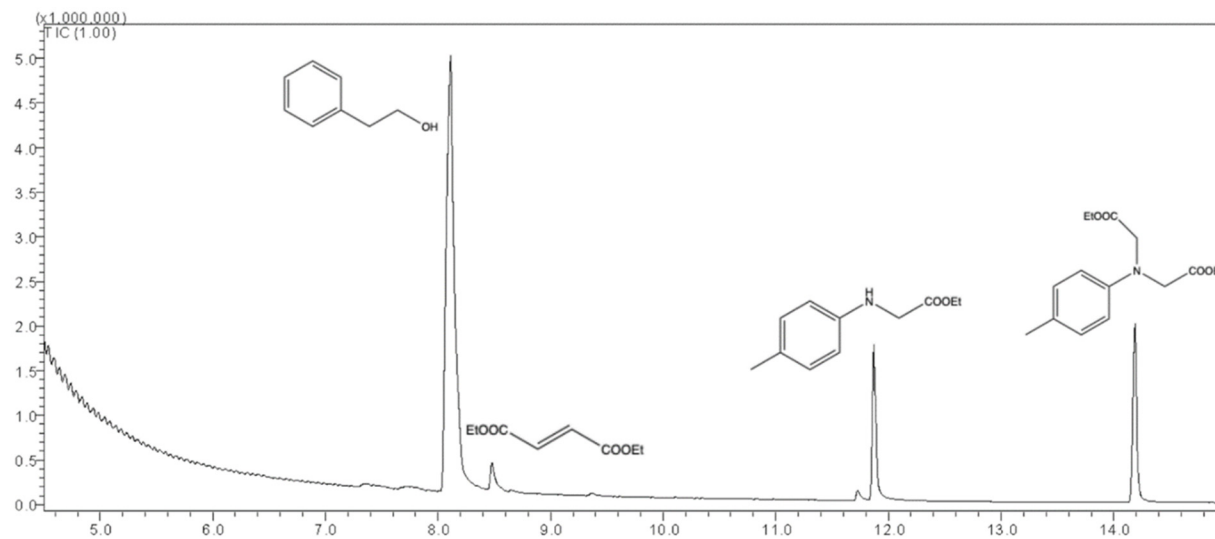
Molecular Weight: 161.13



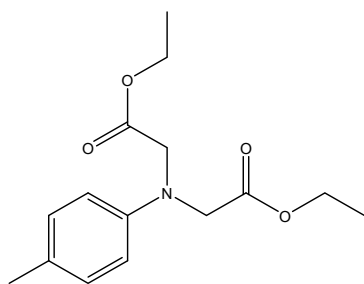
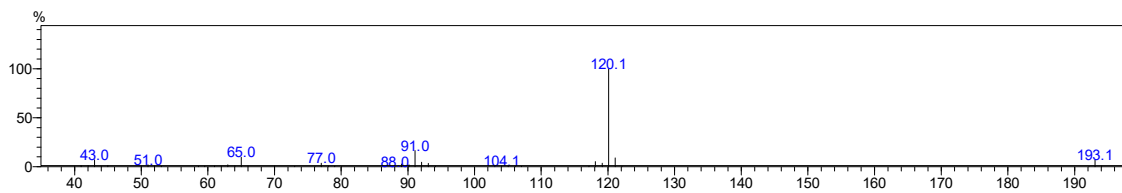
Molecular Weight: 247.22



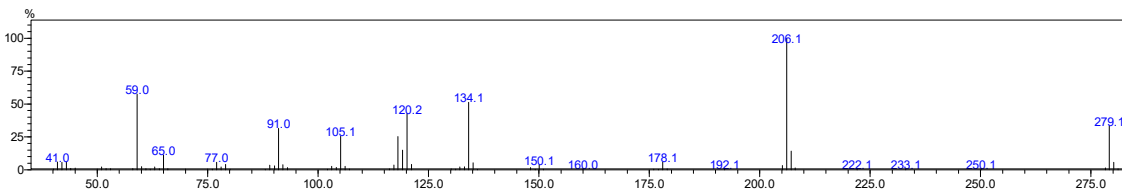
p-Toluidine



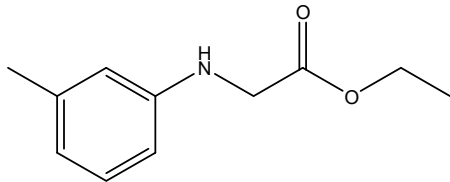
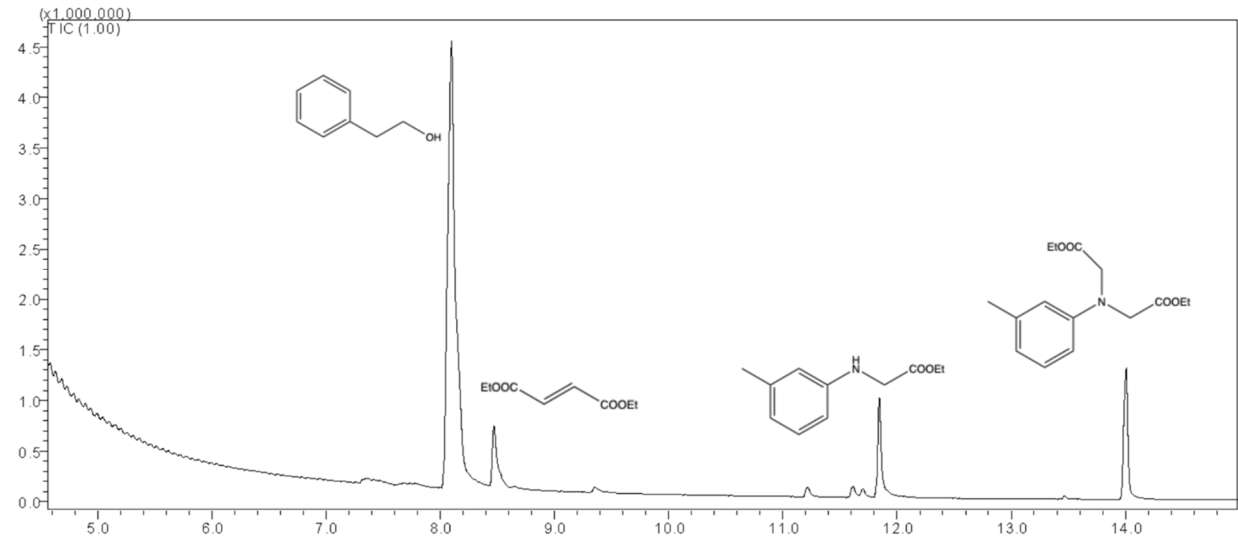
Molecular Weight: 193.25



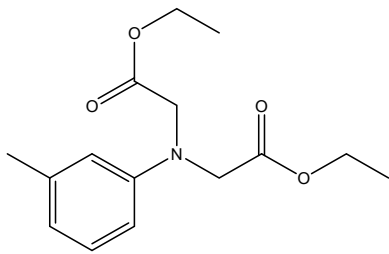
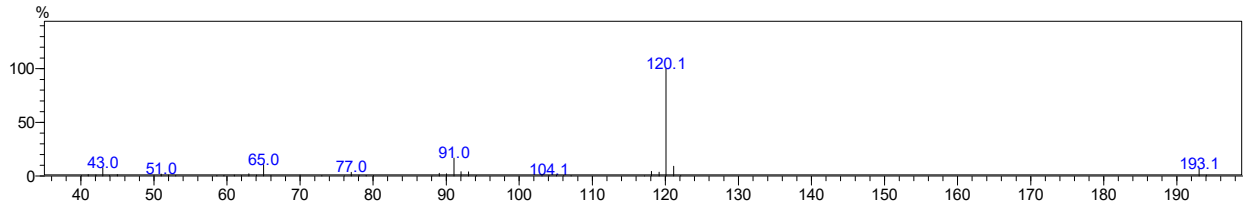
Molecular Weight: 279.34



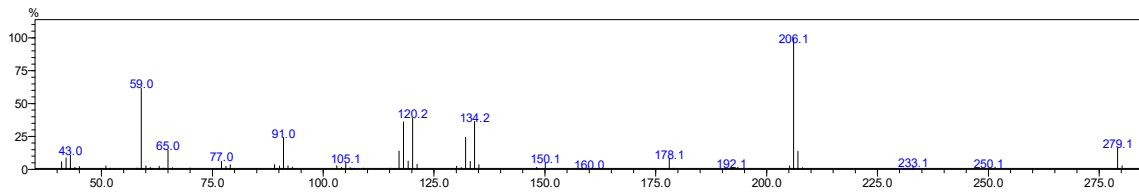
m-Toluidine



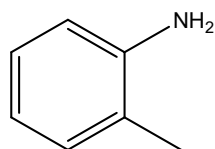
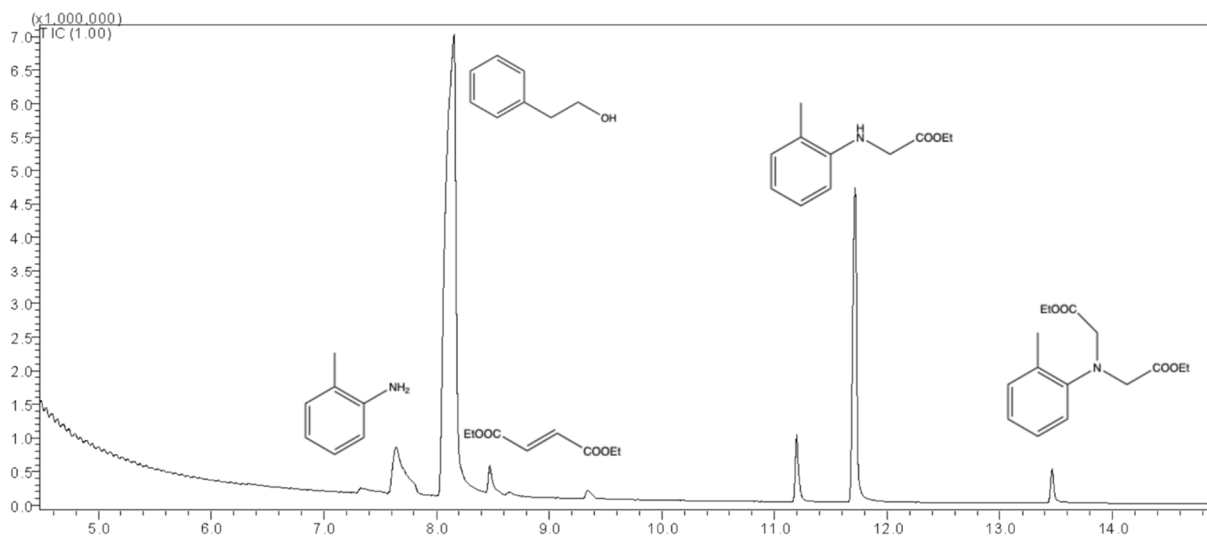
Molecular Weight: 193.25



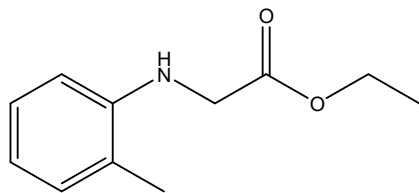
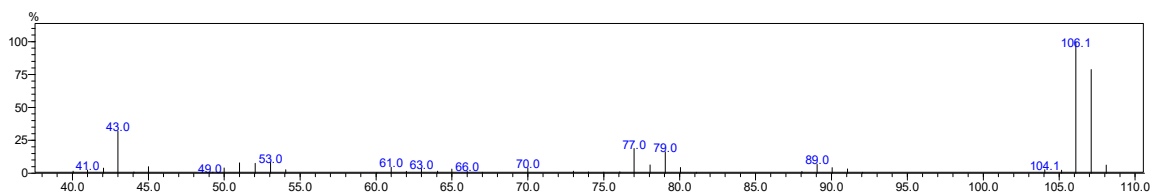
Molecular Weight: 279.34



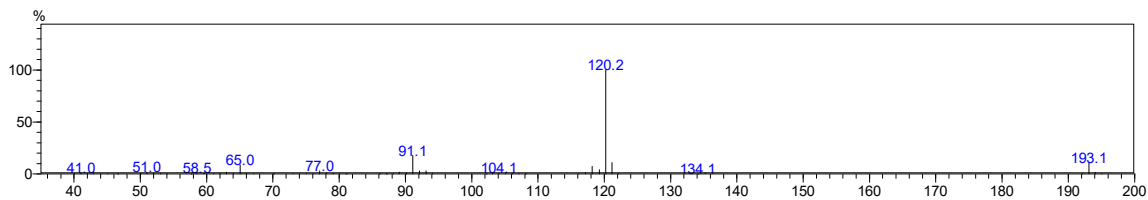
***o*-Toluidine**

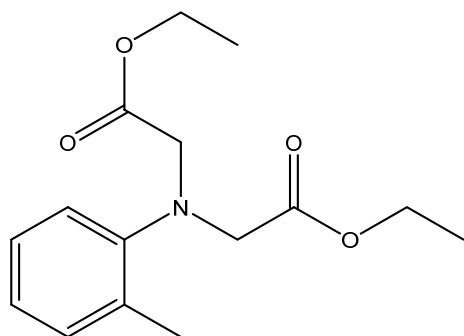


Molecular Weight: 107.16

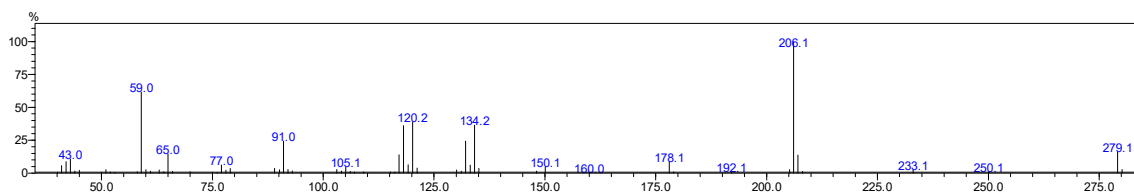


Molecular Weight: 193.25

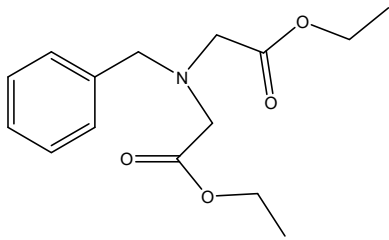
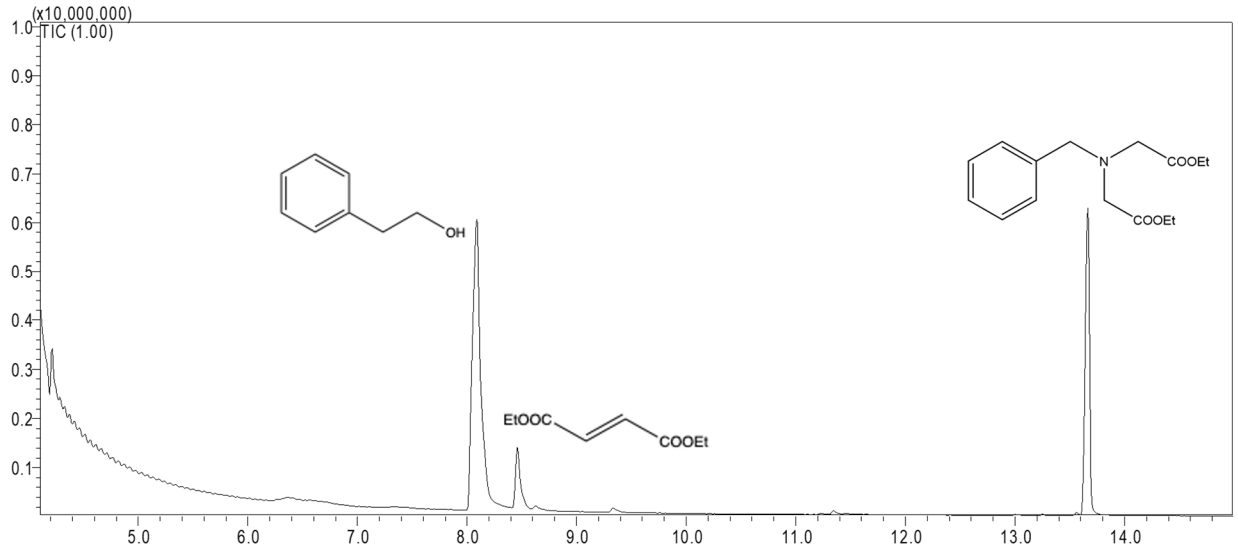




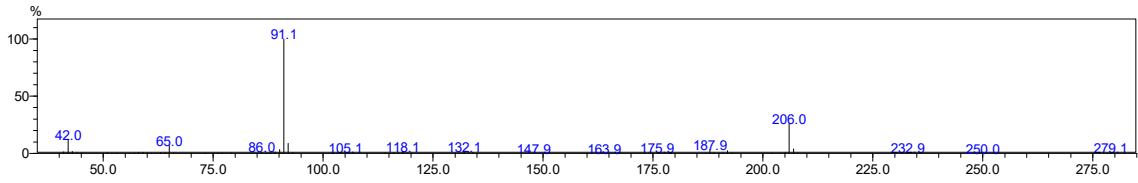
Molecular Weight: 279.34



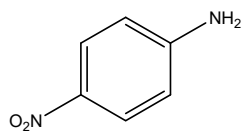
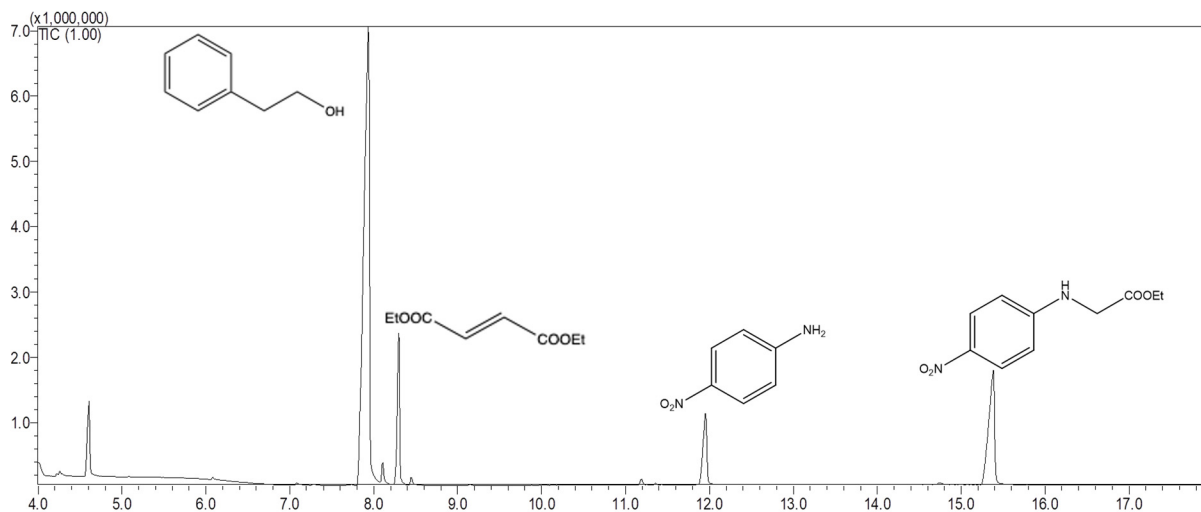
Benzylamine



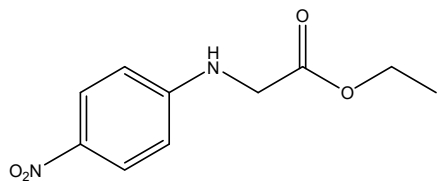
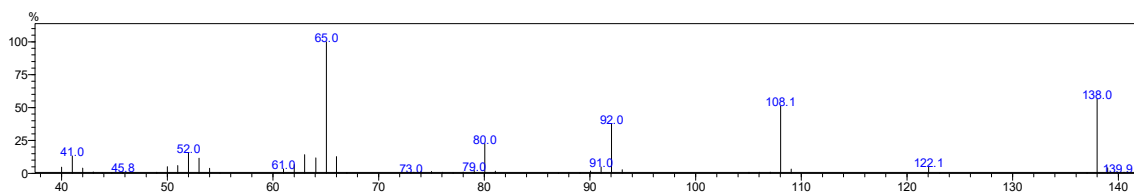
Molecular Weight: 279.34



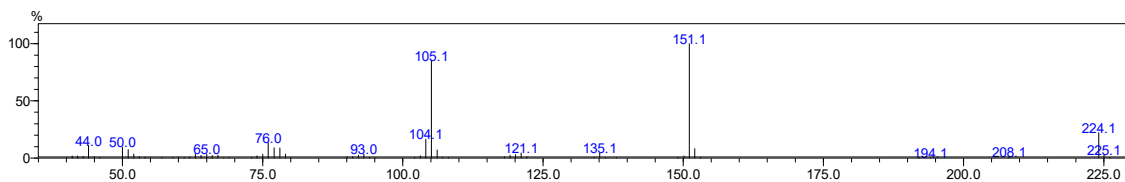
4-Nitroaniline



Molecular Weight: 138.13

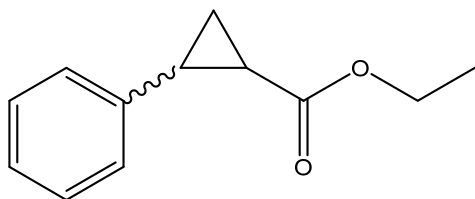
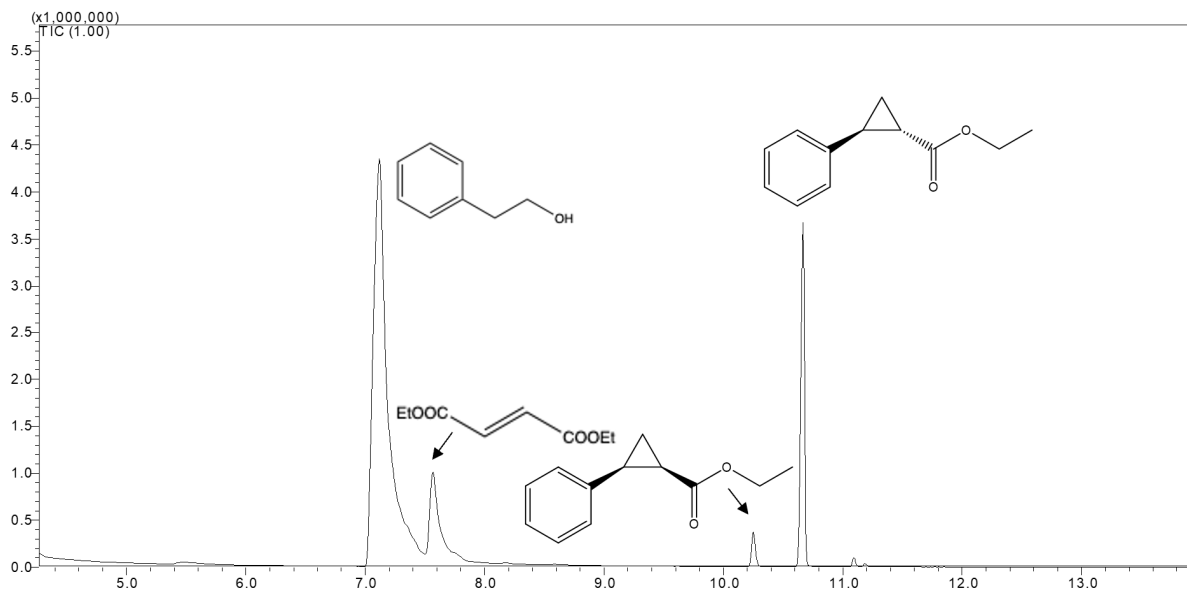


Molecular Weight: 224.22

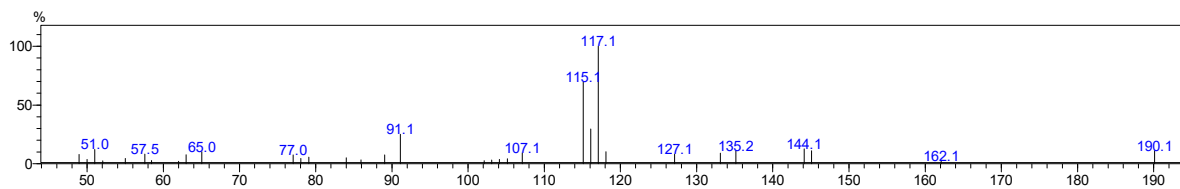


Cyclopropanation Products- GC/MS chromatogram data

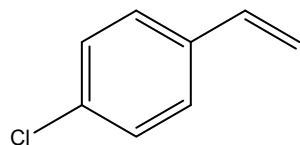
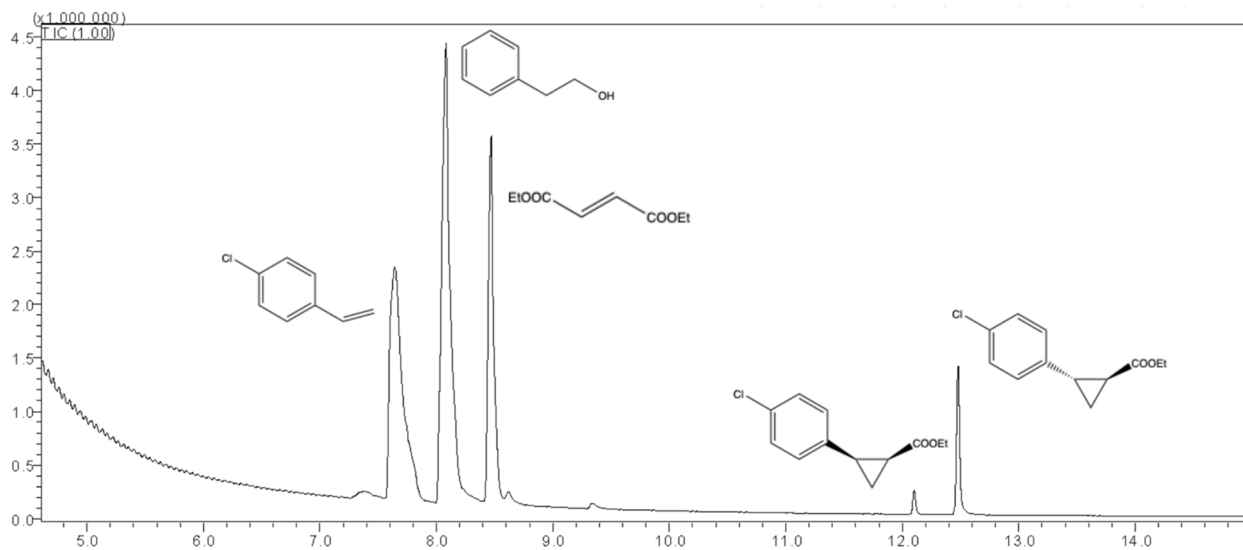
Styrene



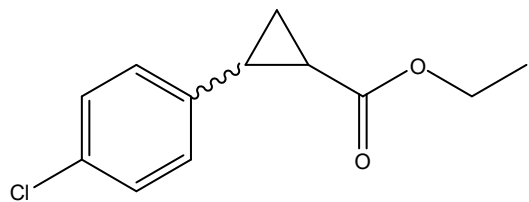
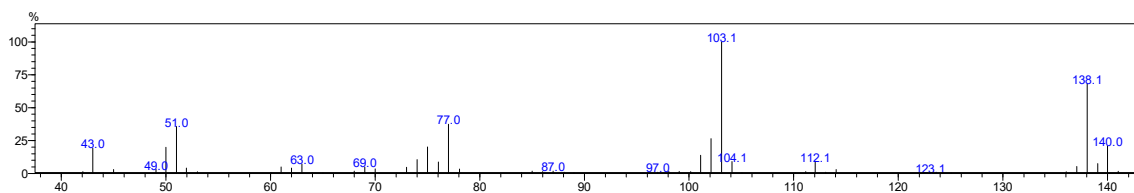
Molecular Weight: 190.24



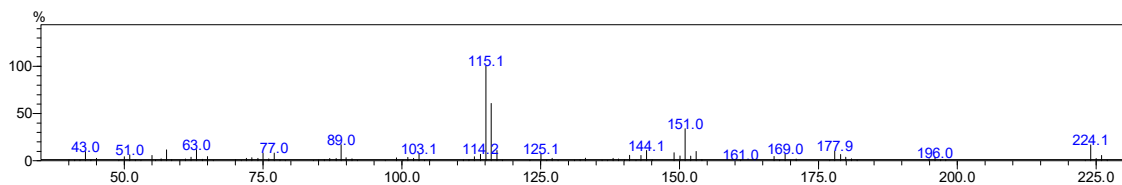
4-Chlorostyrene



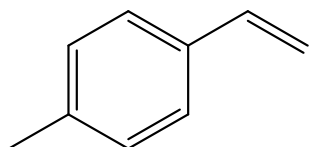
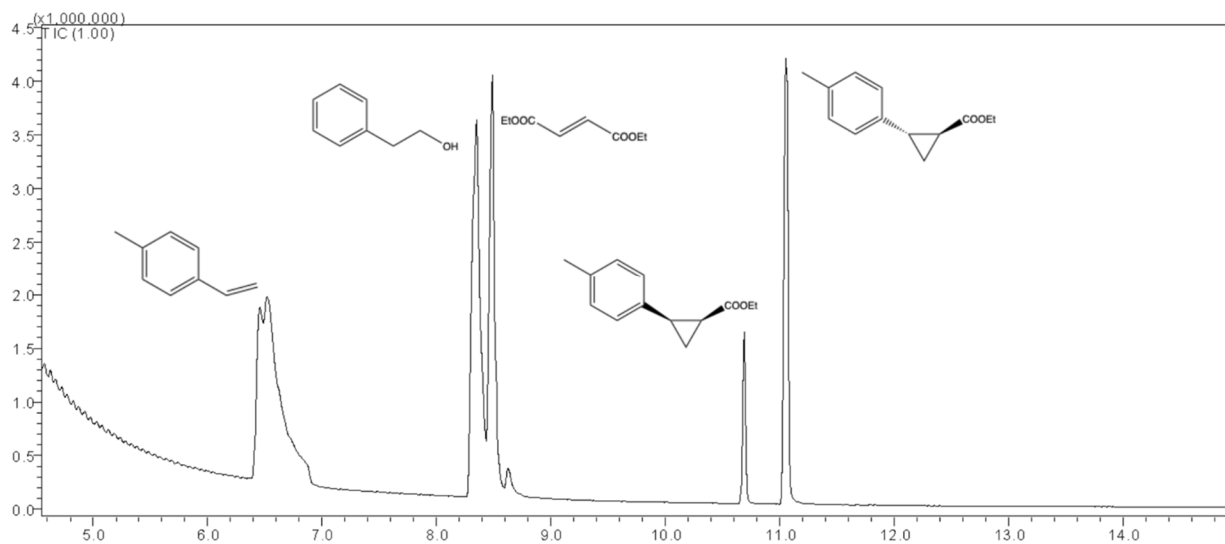
Molecular Weight: 138.59



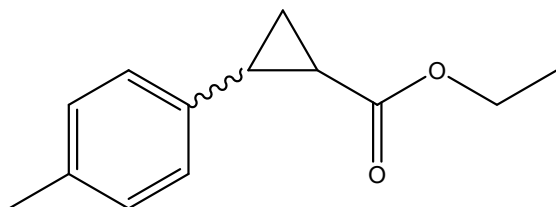
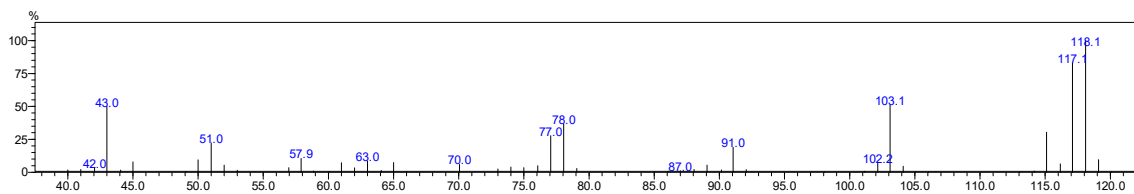
Molecular Weight: 224.68



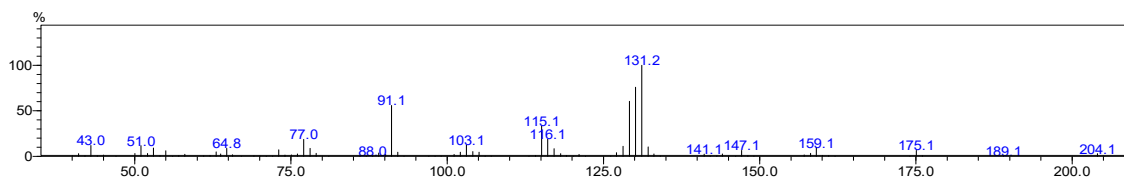
4-Methylstyrene



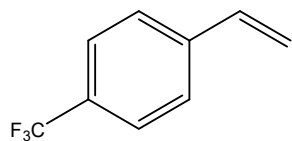
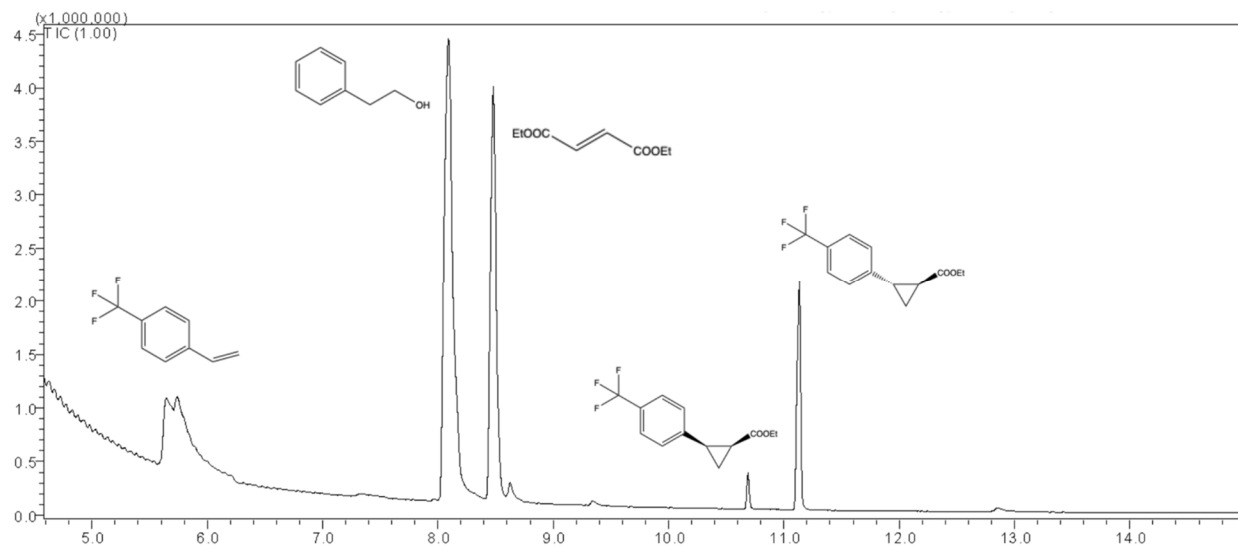
Molecular Weight: 118.18



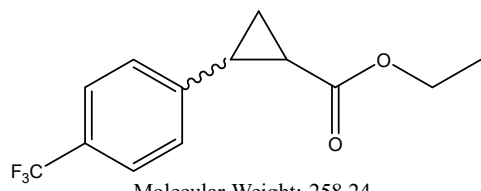
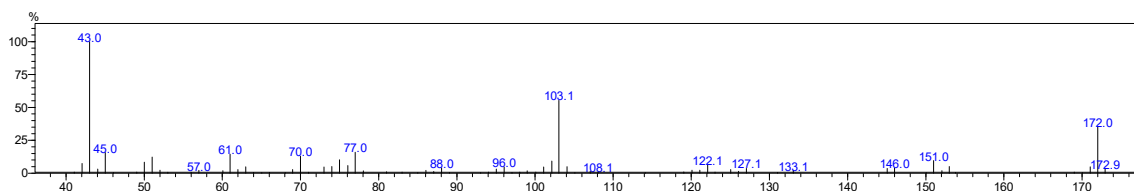
Molecular Weight: 204.27



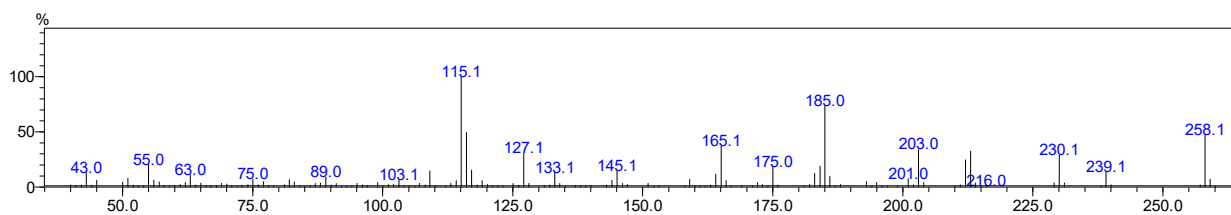
Trifluoromethylstyrene



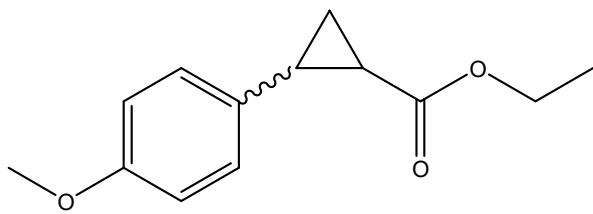
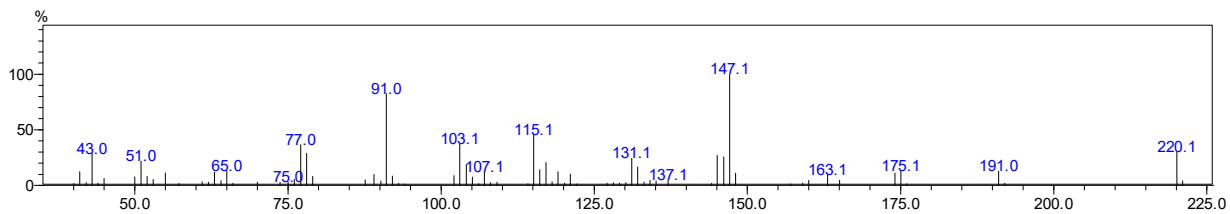
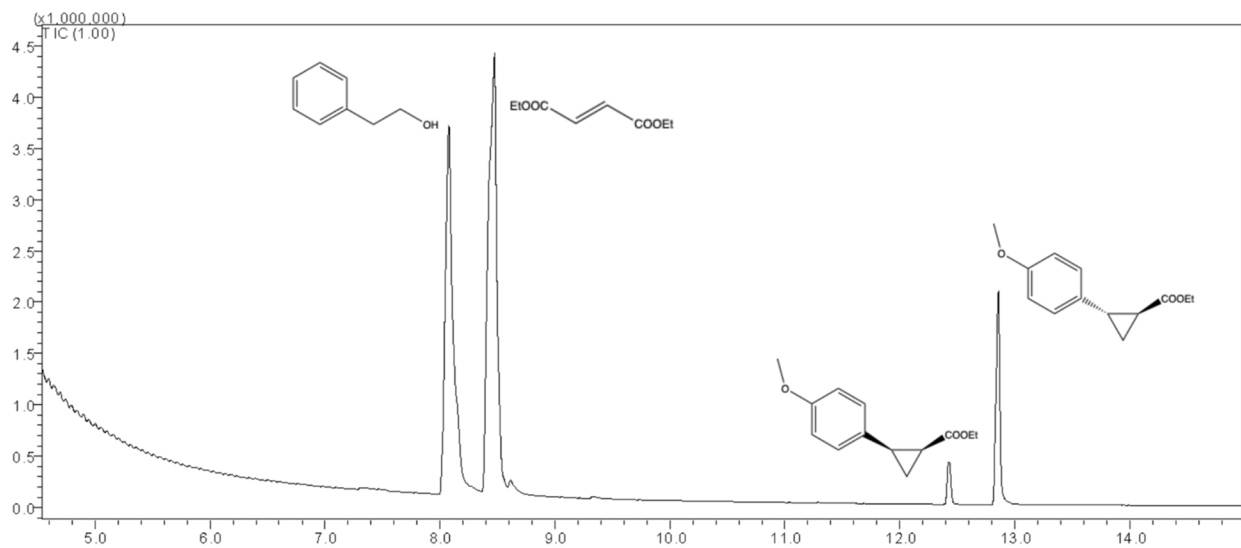
Molecular Weight: 172.15



Molecular Weight: 258.24



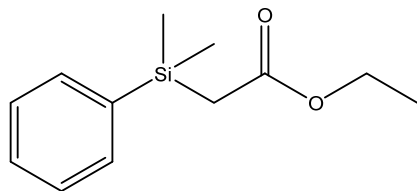
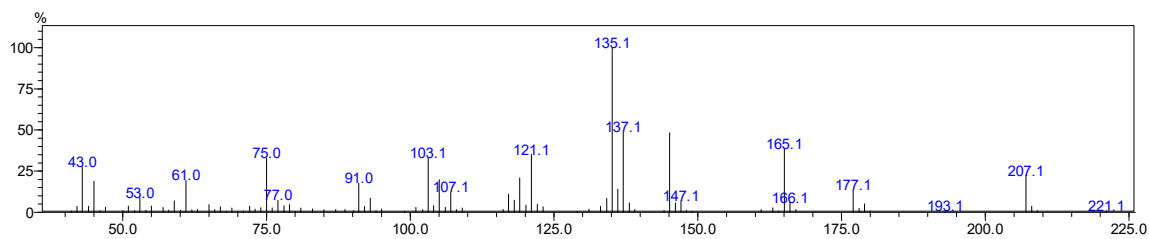
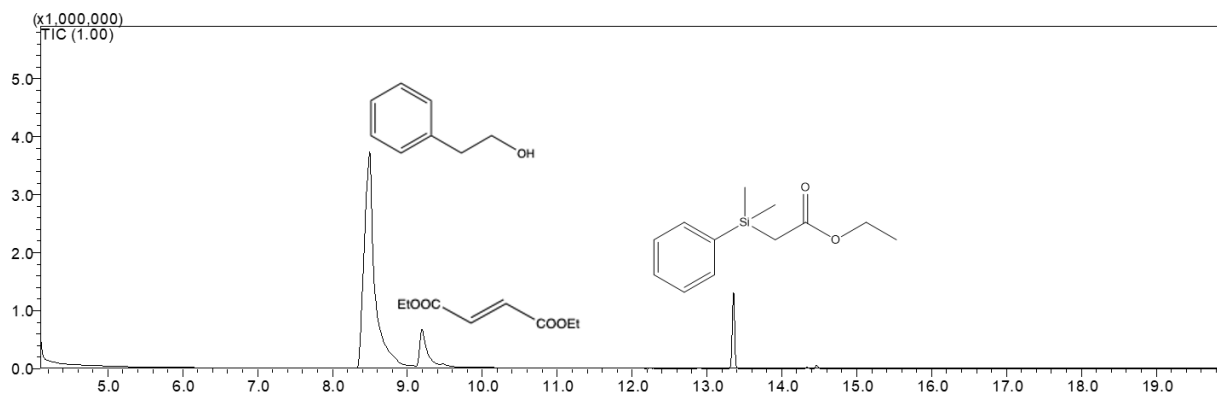
Vinylisole



Molecular Weight: 220.27

Si-H Insertion Products- GC/MS chromatogram data

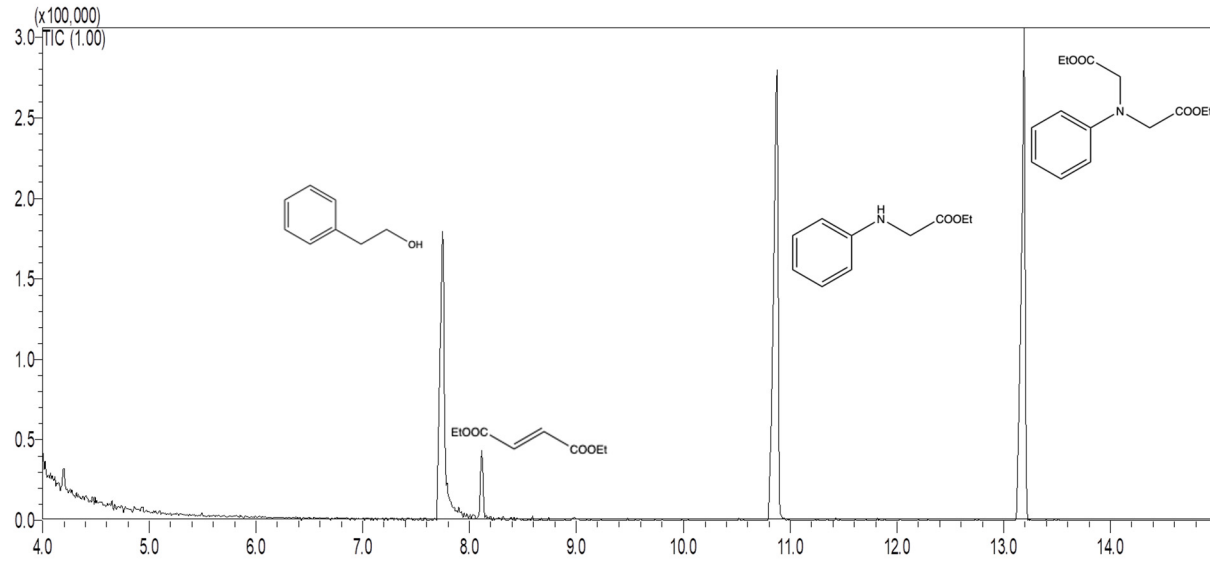
Dimethylphenylsilane



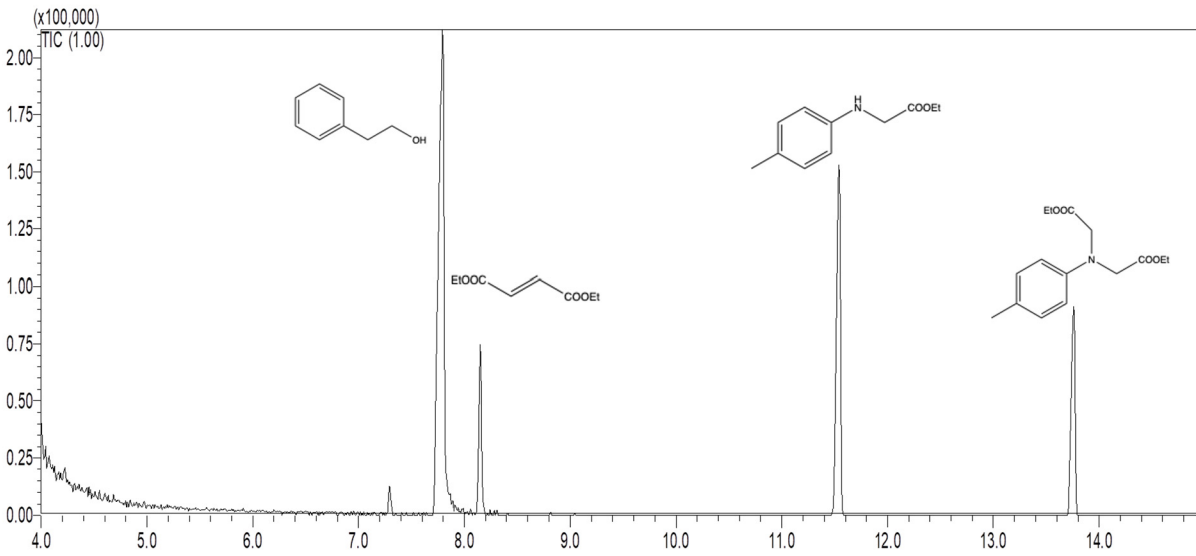
Molecular Weight: 222.36

GC/MS chromatogram data for YfeX R232A

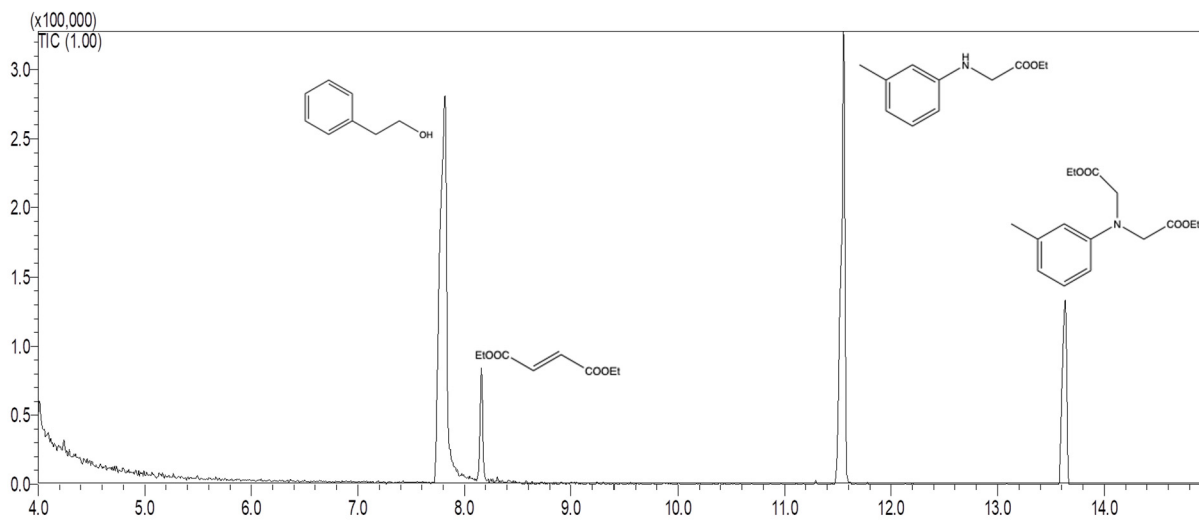
YfeX R232A Aniline



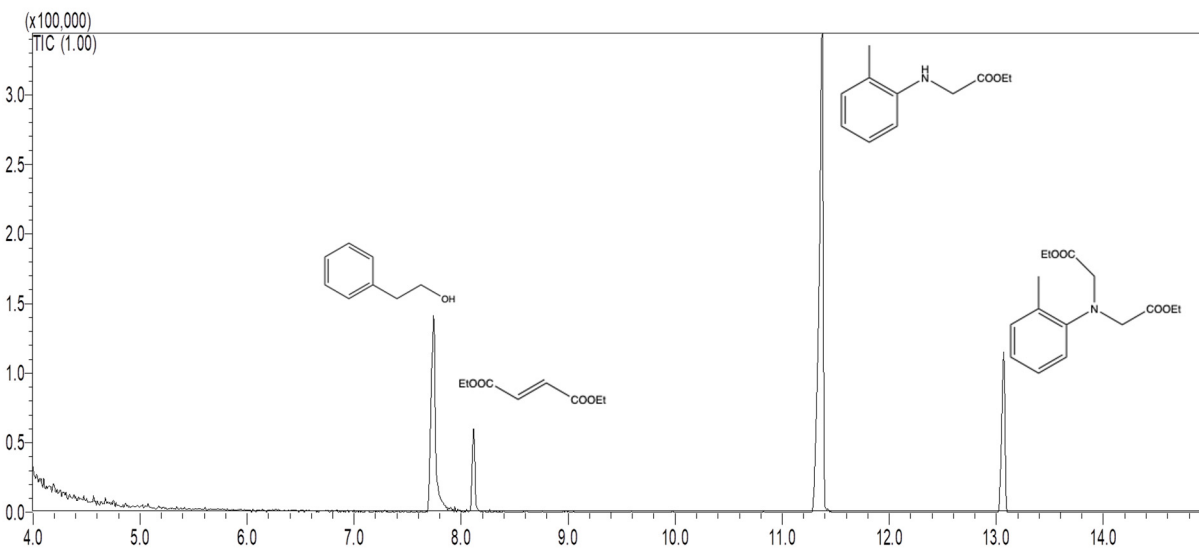
YfeX R232A *para*-toluidine



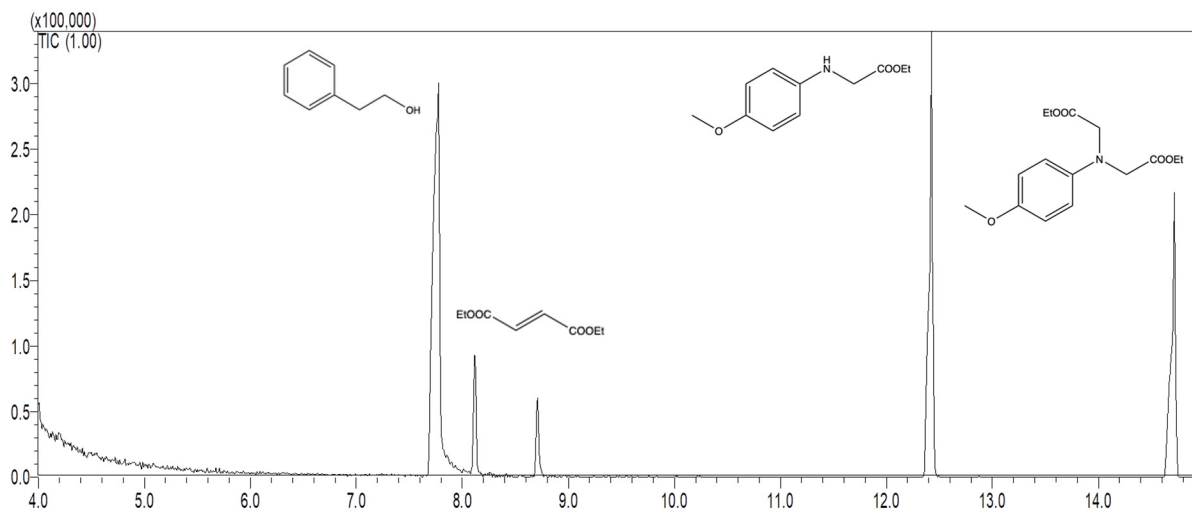
YfeX R232A *meta*-toluidine



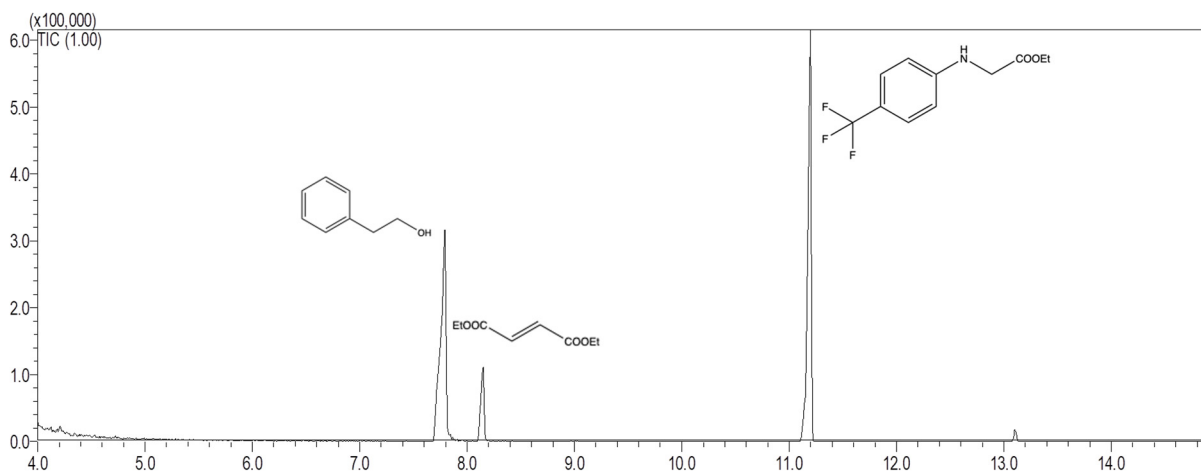
YfeX R232A *ortho*-toluidine



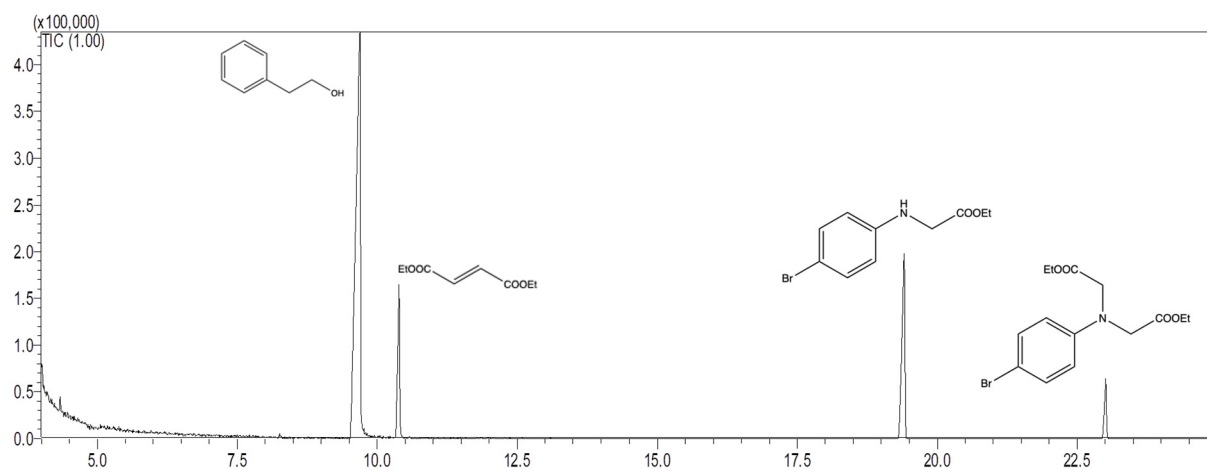
YfeX R232A *para*-anisidine



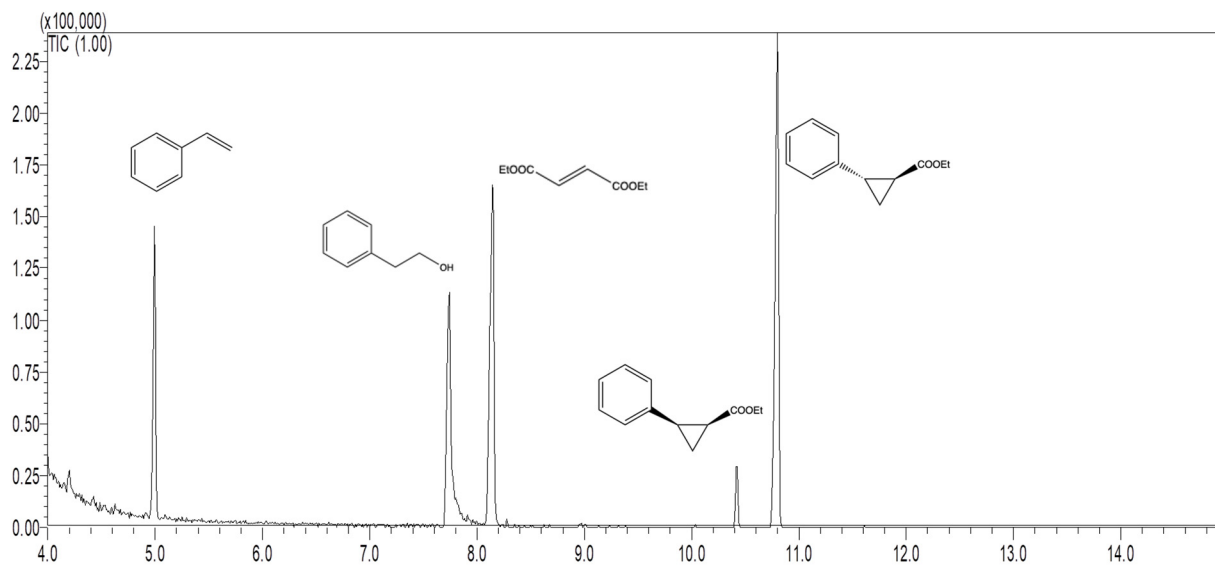
YfeX R232A trifluoromethyl aniline



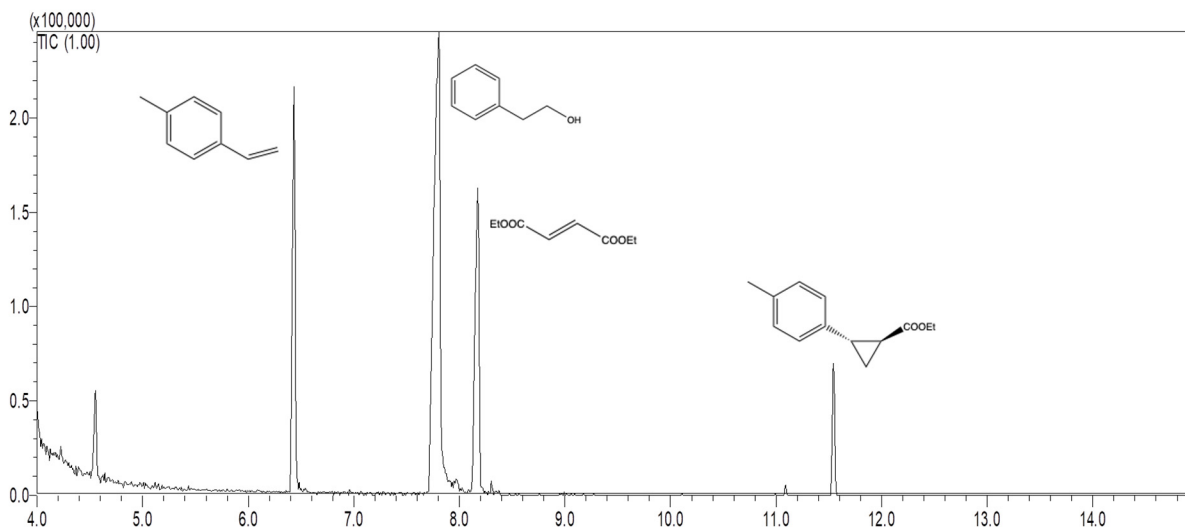
YfeX R232A bromoaniline



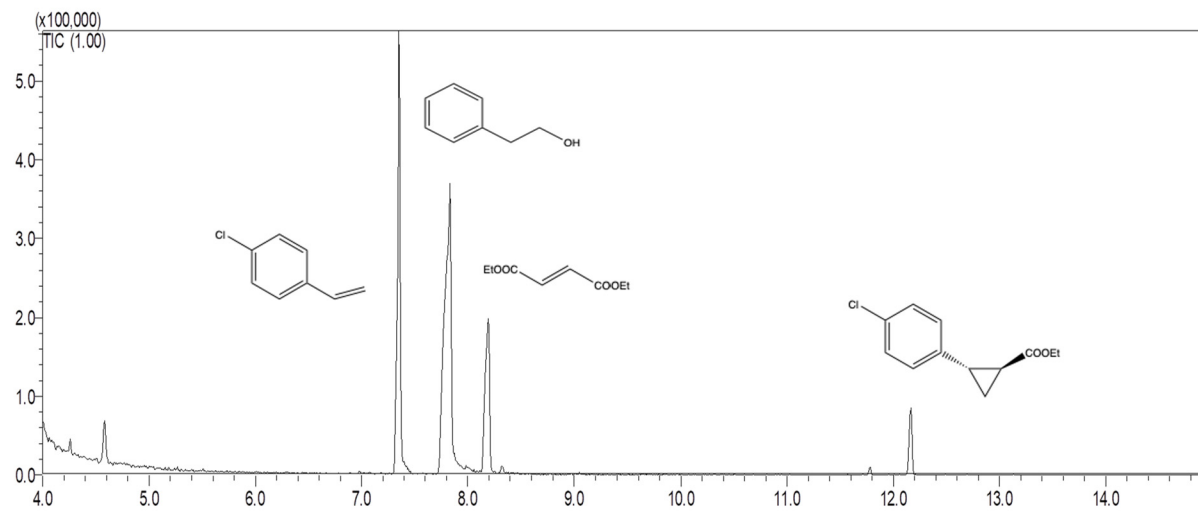
YfeX R232A styrene



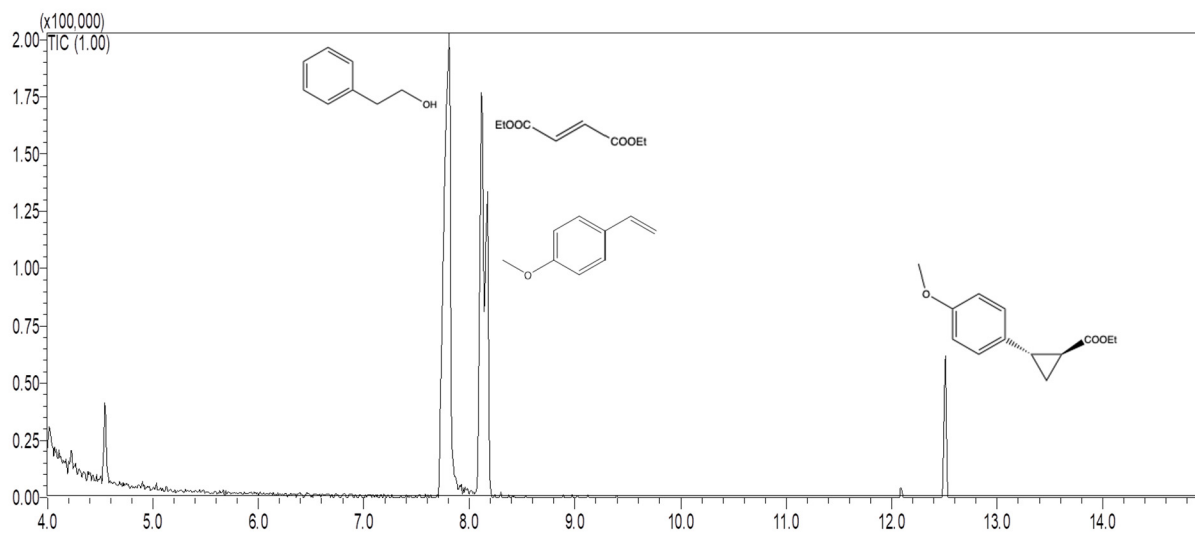
YfeX R232A methylstyrene



YfeX R232A chlorostyrene

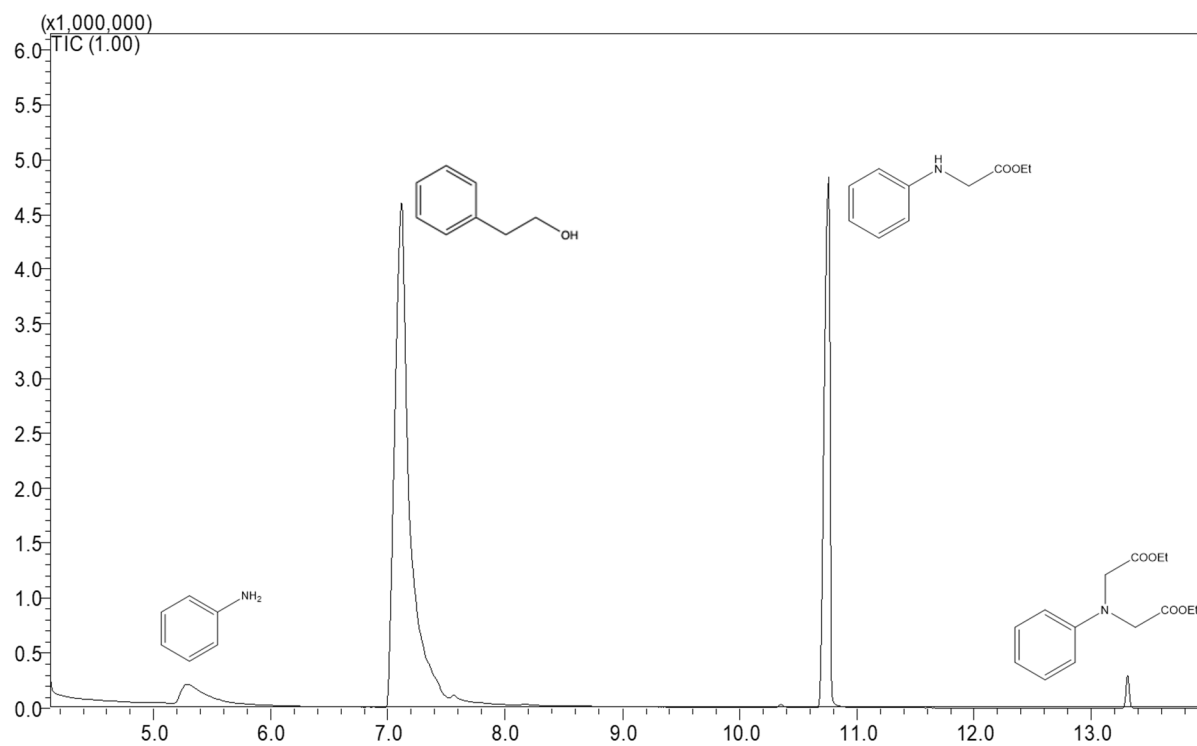


YfeX R232A vinylanisole

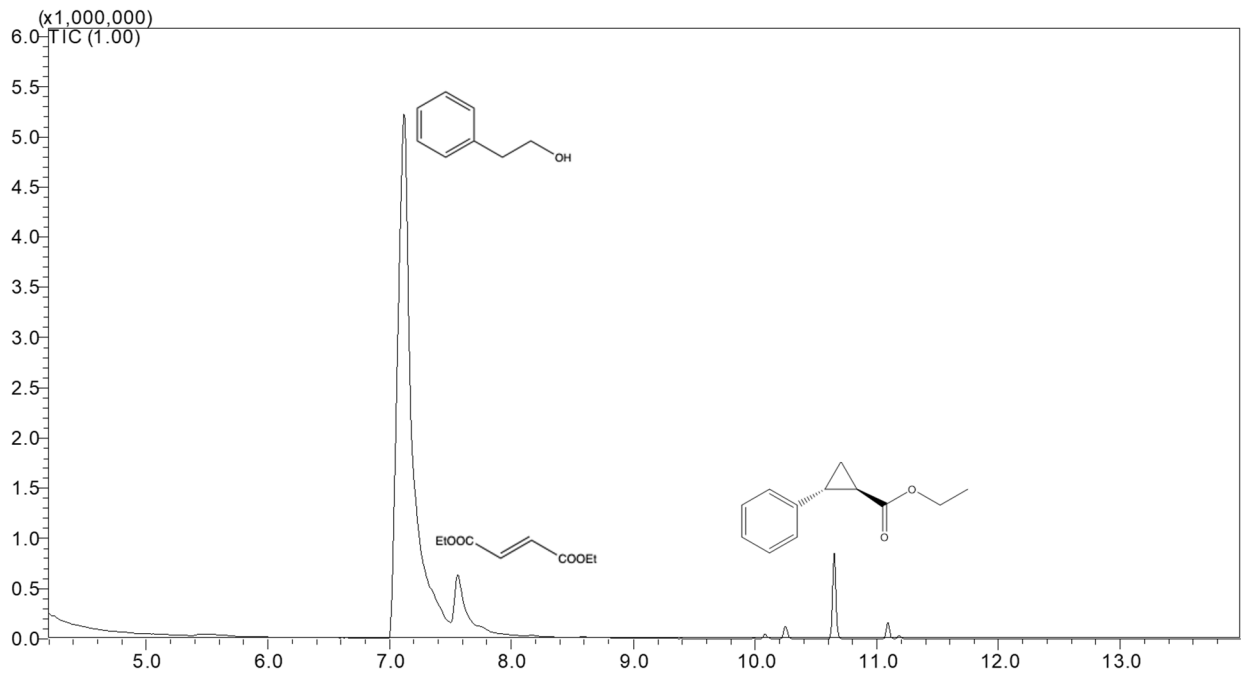


GC/MS chromatogram data for RuYfeX

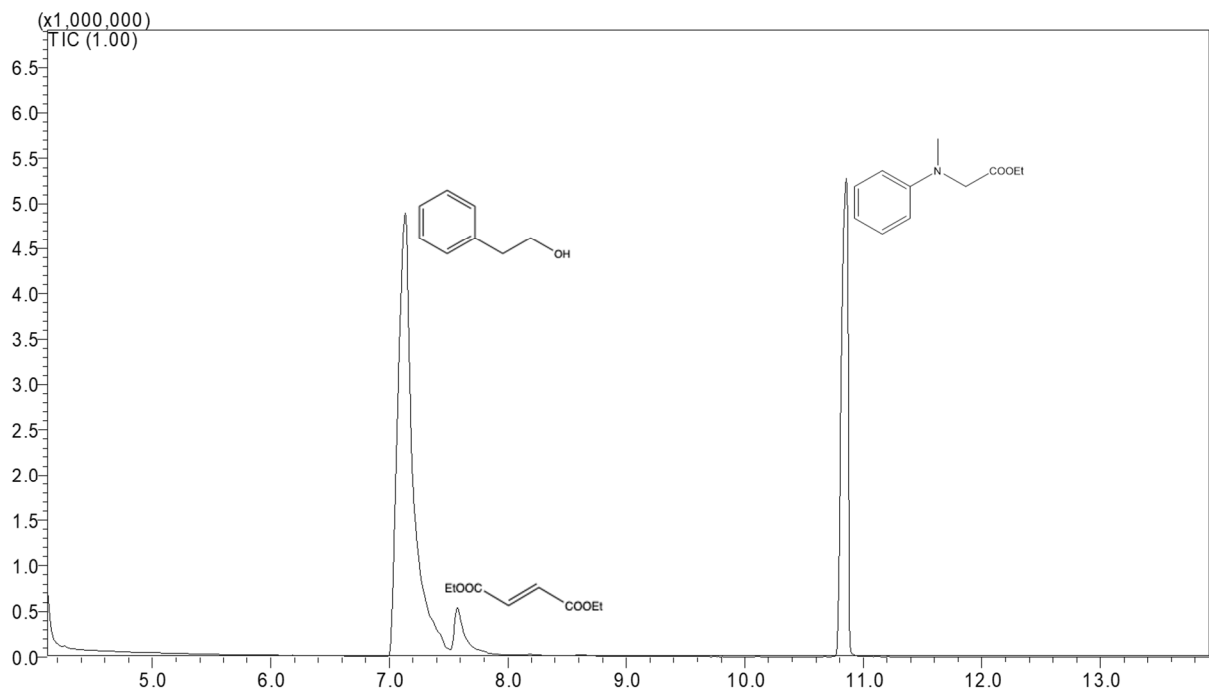
RuYfeX Aniline



RuYfeX Styrene

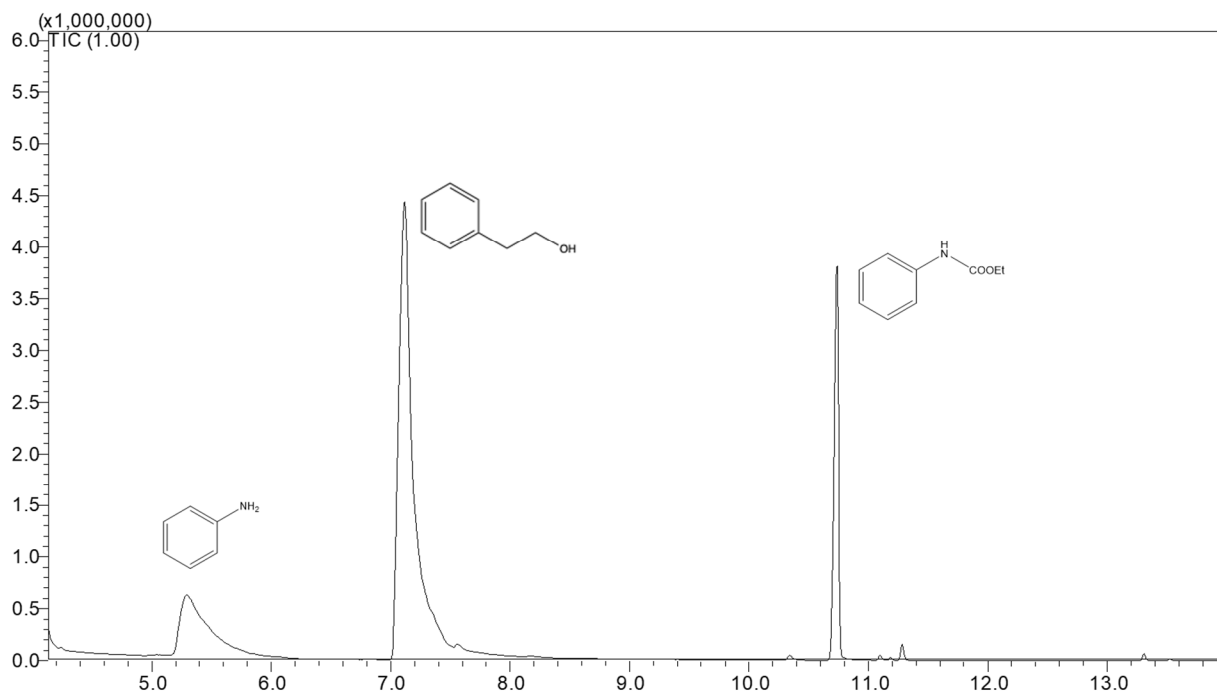


RuYfeX N-methylaniline

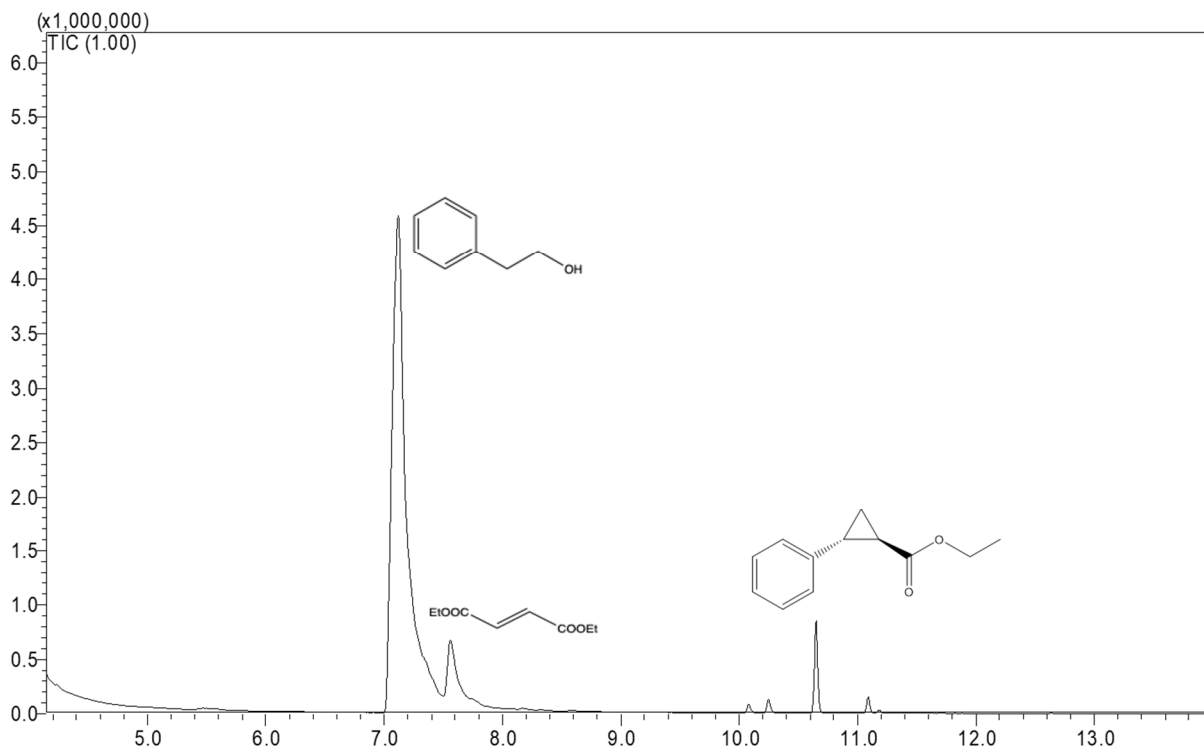


GC/MS chromatogram data for CoYfeX

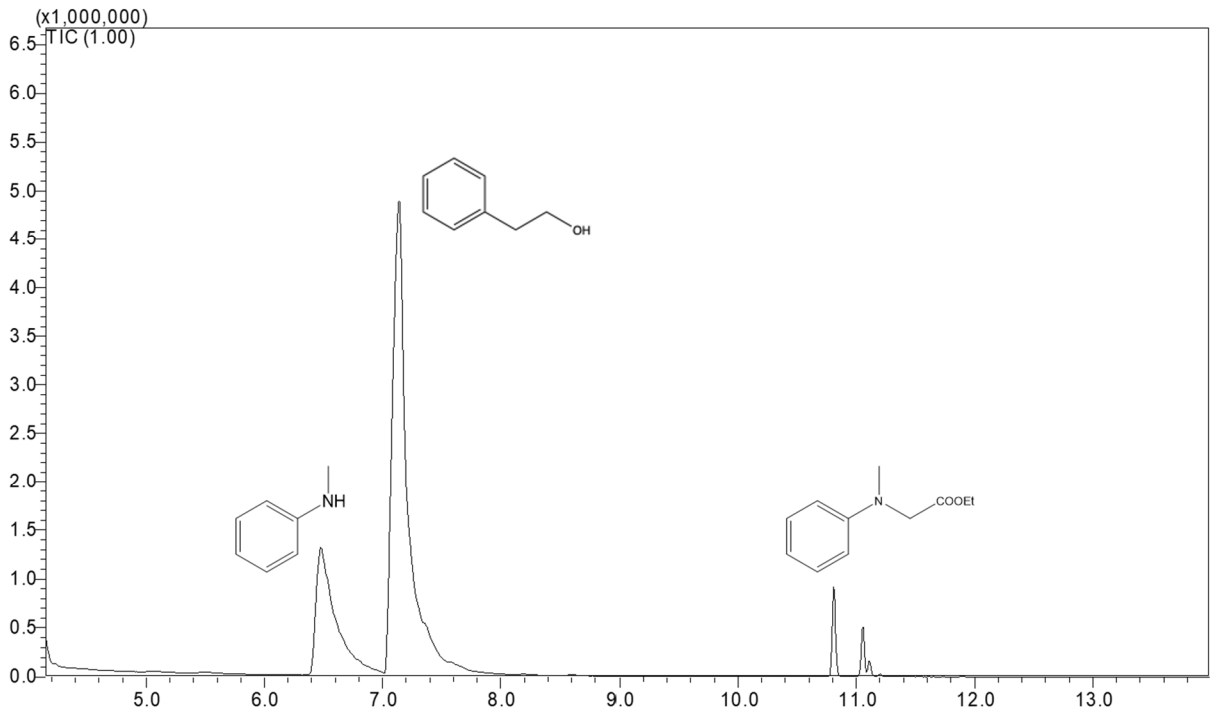
CoYfeX Aniline



CoYfeX Styrene



CoYfeX N-methylaniline



20 mg Large scale reaction:

YfeX Aniline

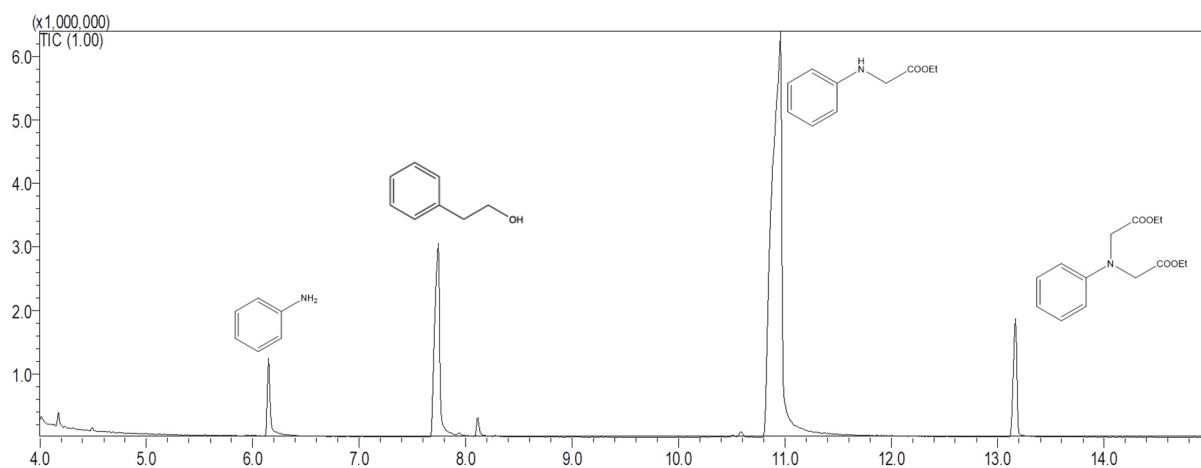


Figure S12. Reactions were performed as previously described for the 10 mL scale using 20 μ M YfeX, 20 mM aniline, 20 mM ethyl diazoacetate (EDA), and 10 mM $\text{Na}_2\text{S}_2\text{O}_4$. The sodium dithionite (100 mM stock solution) in potassium phosphate buffer (100 mM, pH 7.0) was purged by bubbling nitrogen through the solution for 10 min in a sealed vial, with a total MeOH content of 2.65%. All reagents and proteins were brought into a Coy vinyl anaerobic chamber (10–30 ppm of O_2 , 1.5–3.0% H_2) before running the reactions. The reactions were left under magnetic agitation for 1 h at room temperature. The reactions were analyzed, as previously described, by addition of internal standard (2-phenyl-ethanol, 1 M in methanol) to the reaction mixture, followed by extraction with 30 mL of ethyl acetate. The organic layers were dried with magnesium sulfate and later filtered and analyzed by GC/MS (see General Procedures section for details on GC/MS analyses). Based on a calibration curve and internal standard we obtained a total yield of 65–69% (duplicate reactions).

Substrate Ratios

1:4 (EDA: Aniline)

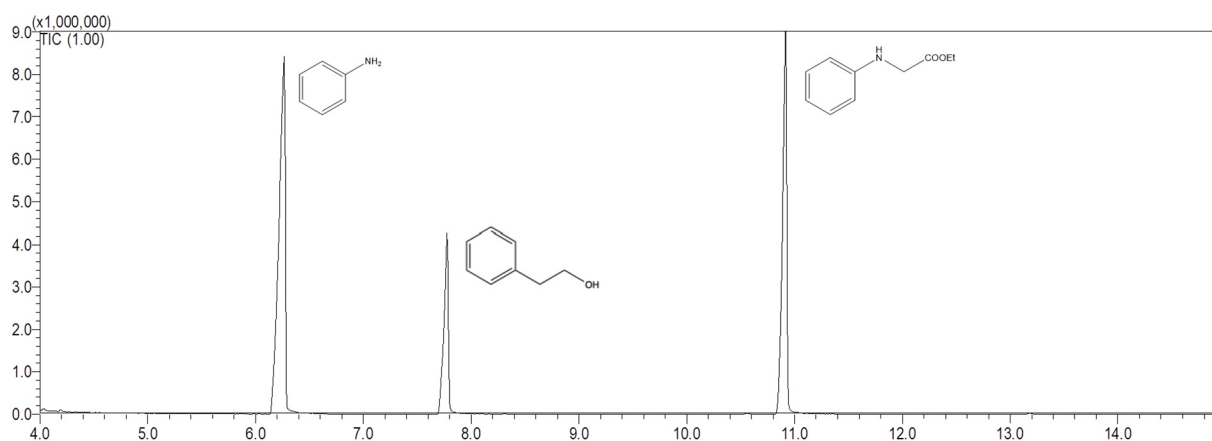


Figure S13. GC/MS traces of substrate optimization of the N–H insertion reaction of aniline catalyzed by YfeX. Reaction conditions: 20 μ M YfeX (0.1 mol%), 40 mM aniline, 10 mM EDA, 10 mM dithionite, 1 hour reaction time in 50 mM phosphate buffer (pH 7.4). Yield: $79.3 \pm 12\%$ with a mono-:disubstitution ratio of 99.67:0.33.

4:1 (EDA: Aniline)

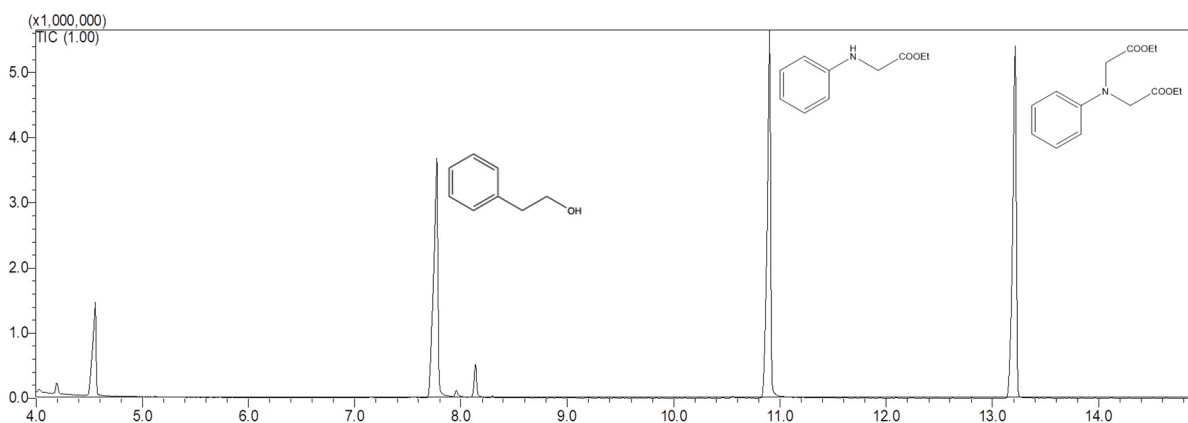


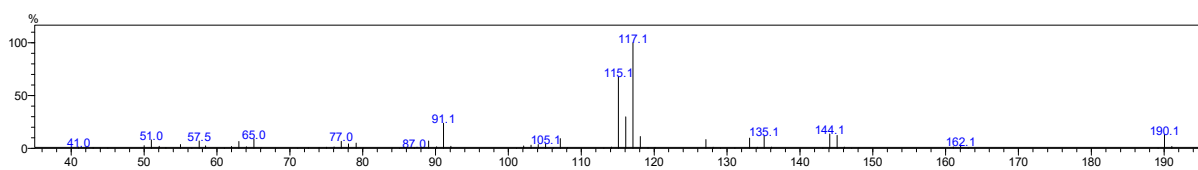
Figure S14. GC/MS traces of substrate optimization of the N–H insertion reaction of aniline catalyzed by YfeX. Reaction conditions: 20 μ M YfeX (0.1 mol%), 10 mM aniline, 40 mM EDA, 10 mM dithionite, 1 hour reaction time in 50 mM phosphate buffer (pH 7.4). Yield: $75.6 \pm 11\%$ with a mono-:disubstitution ratio of 48.7:51.3.

Styrene YfeX reaction analysis with supercritical fluid chromatography:

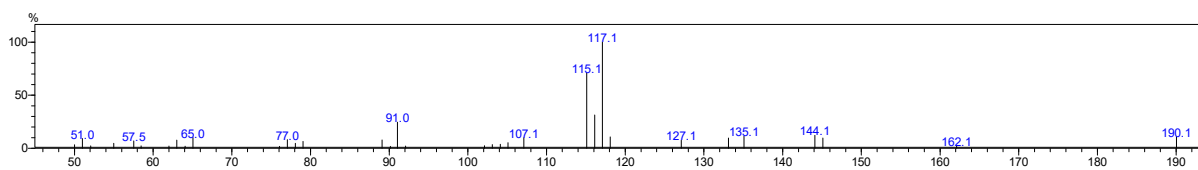
(A)



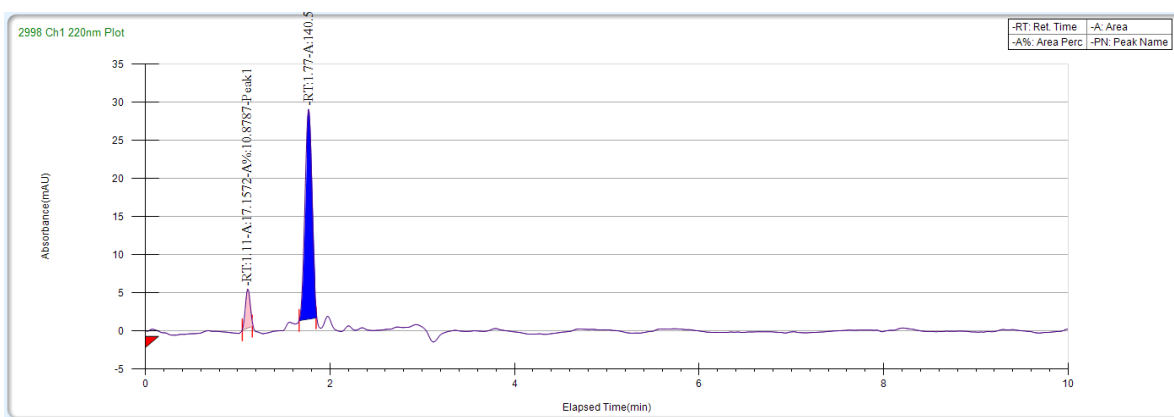
13.69min



13.05min



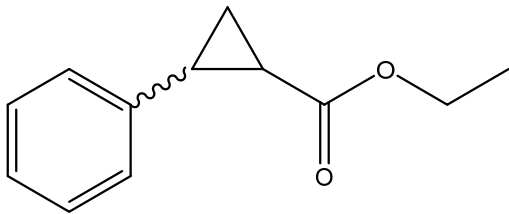
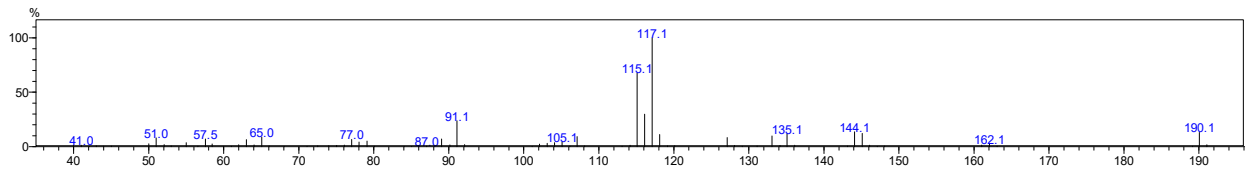
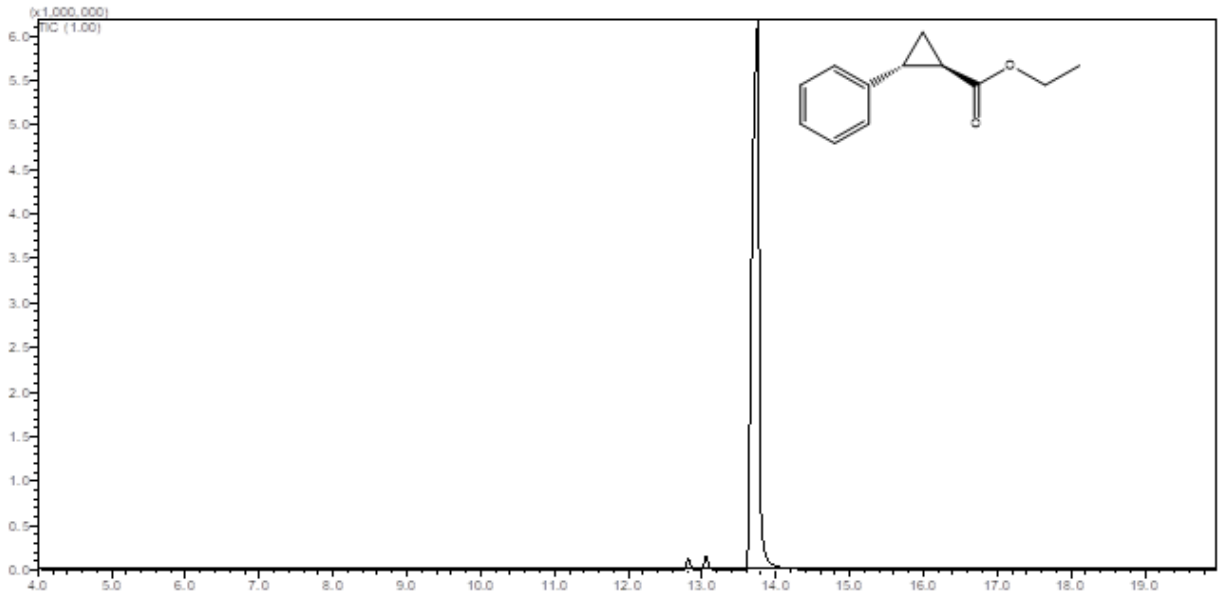
(B)



Peak Name	Area Percent	Area	Retention Time	Height
Peak1	10.8787	17.1572	1.11 min	5.1014
Peak2	89.1213	140.5565	1.77 min	27.5271

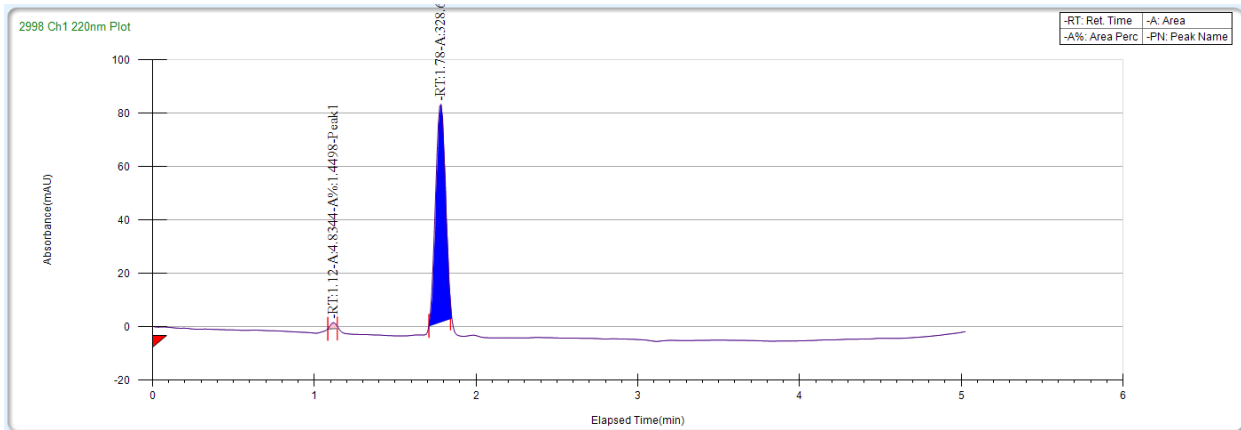
Figure S15. Product analysis for the reaction of YfeX with EDA and styrene, followed by (A) GC/MS and (B) SCF detection using a IC Daicel 5uM 4.6 x 250 mm analytical chiral column, with 10% isopropanol, and detection at 220 nm.

(A)



Molecular Weight: 190.24

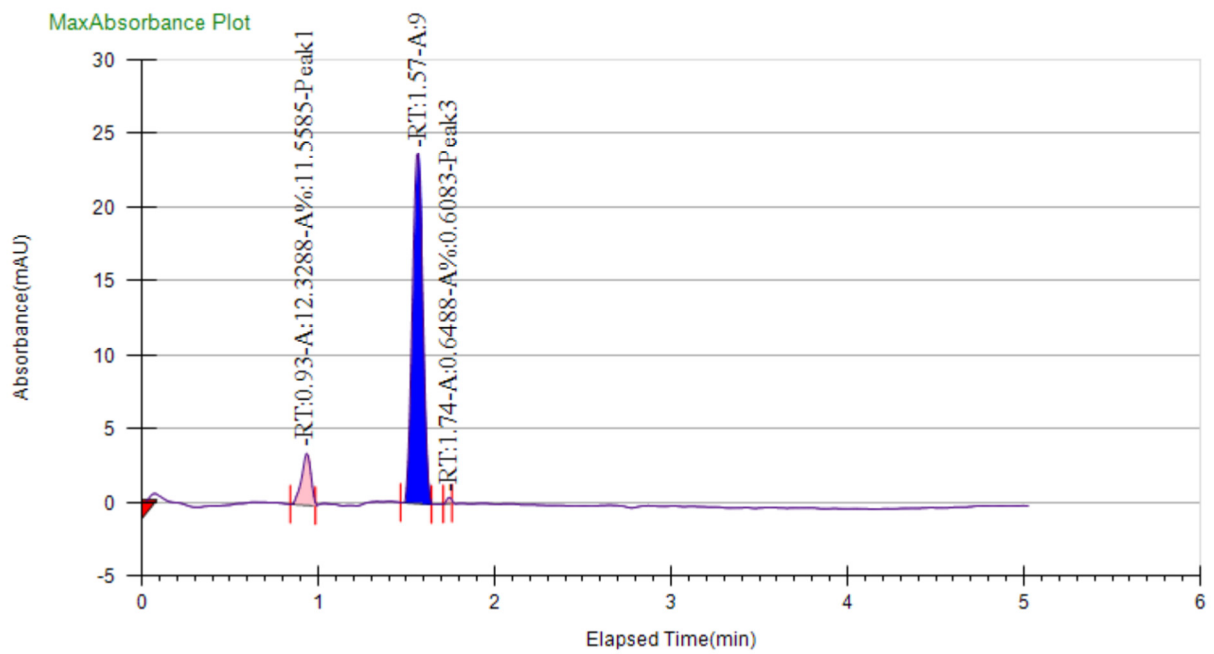
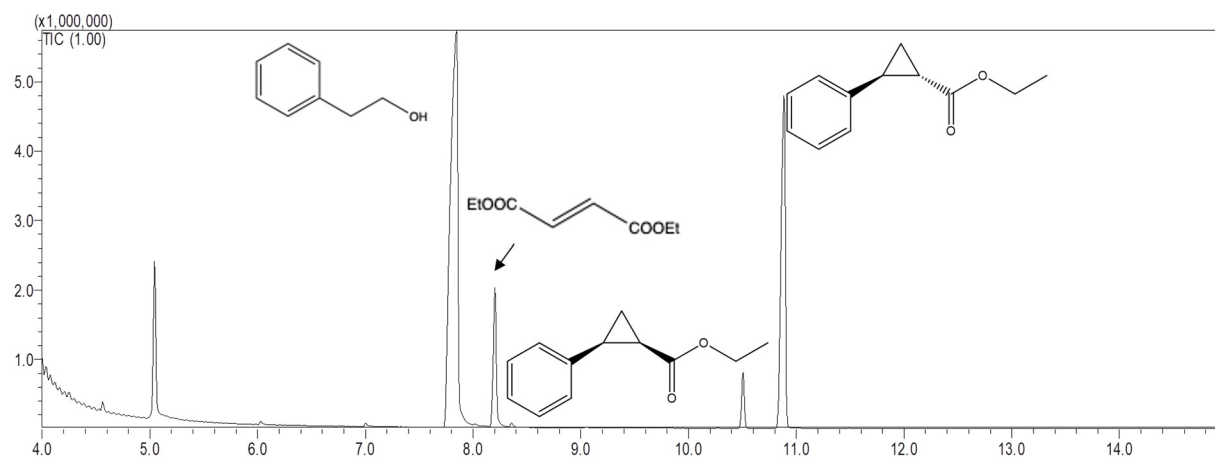
(B)



Peak Name	Area Percent	Area	Retention Time	Height
Peak1	1.4498	4.8344	1.12 min	2.2539
Peak2	98.5502	328.609	1.78 min	81.5001

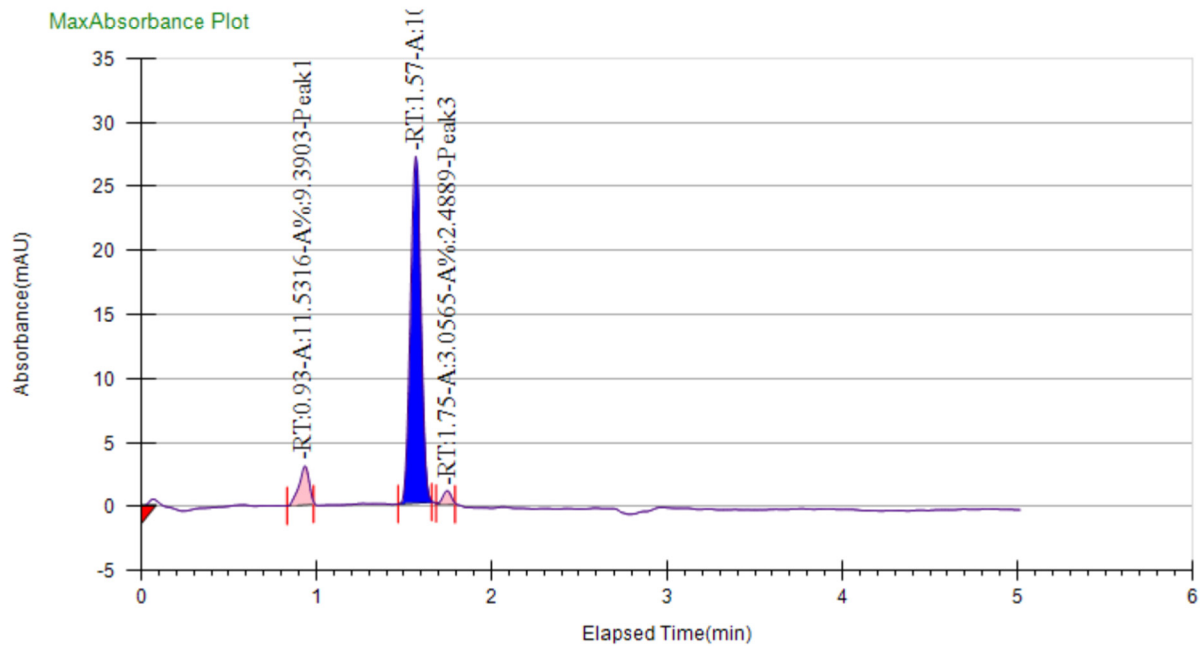
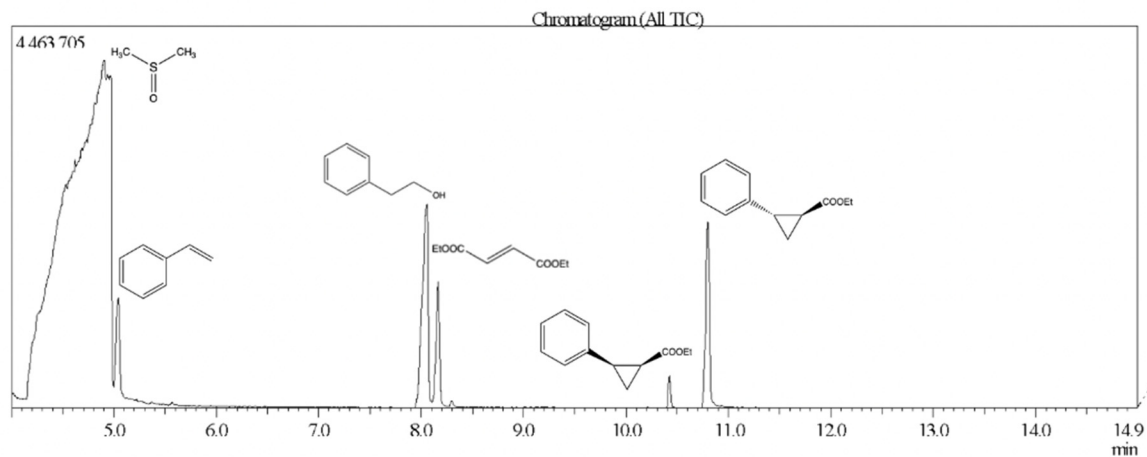
Figure S16. Standard analysis of ethyl (R,R)-2-phenylcyclopropanecarboxylate for the reaction of YfeX with EDA and styrene, followed by (A) GC/MS and (B) SCF detection using a IC Daicel 5 μ M 4.6 x 250 mm analytical chiral column, with 10% isopropanol, and detection at 220 nm.

(A)



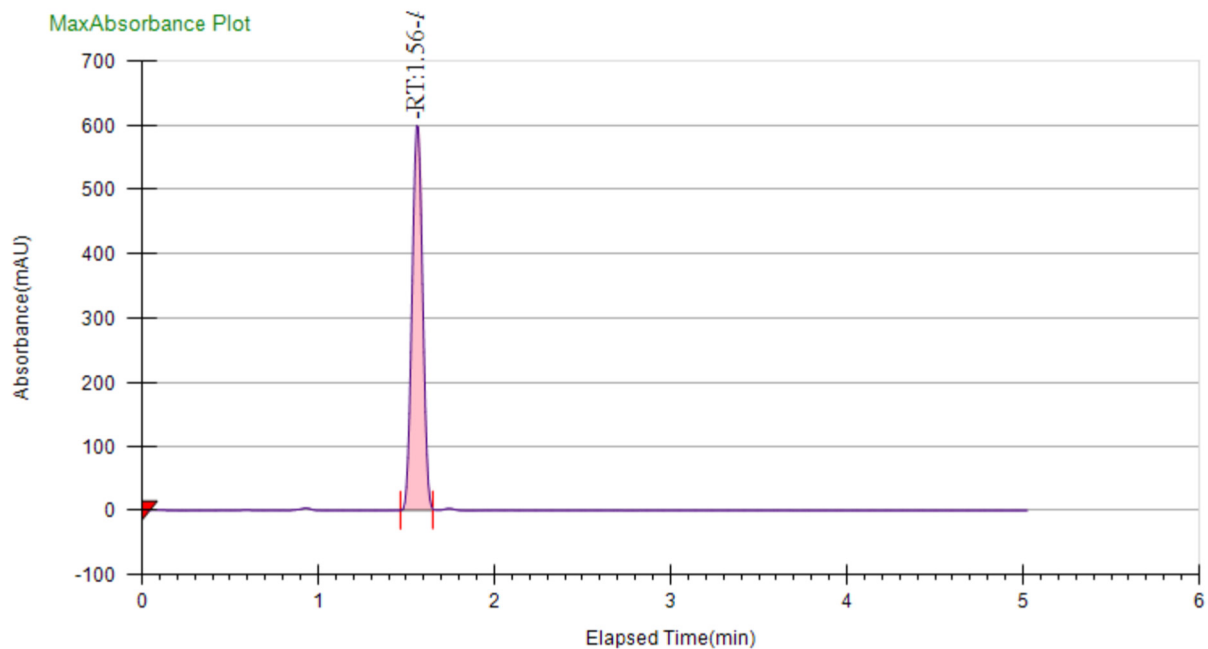
Peak Name	Area Percent	Area	Retention Time	Height
Peak 1	11.5585	12.3288	0.93 min	3.5025
Peak 2	87.8332	93.6867	1.57 min	23.7378
Peak 3	0.6083	0.6488	1.74 min	0.4041

(B)



Peak Name	Area Percent	Area	Retention Time	Height
Peak 1	9.3903	11.5316	0.93 min	3.01
Peak 2	88.1207	108.215	1.57 min	27.0787
Peak 3	2.4889	3.0565	1.75 min	1.027

(C)

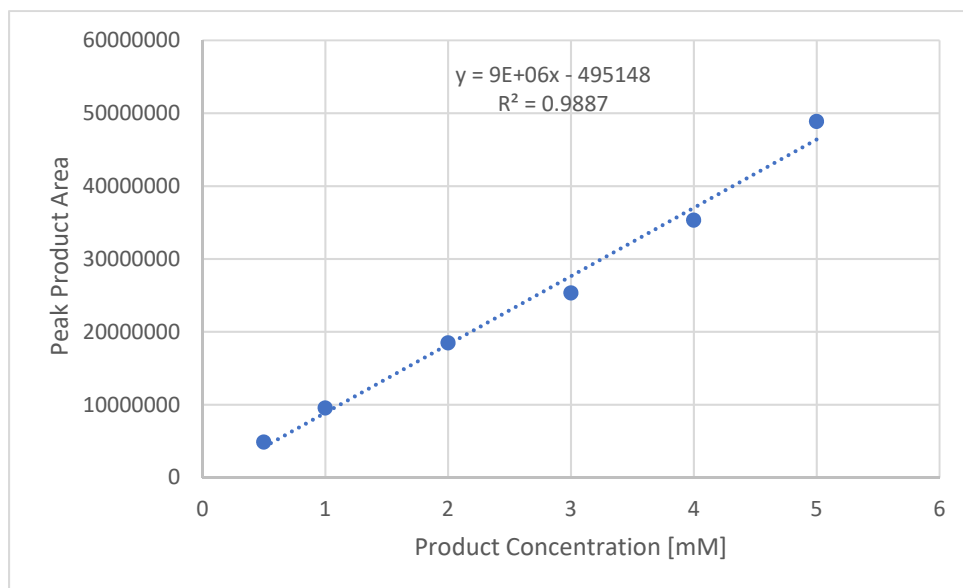


Peak Name	Area Percent	Area	Retention Time	Height
Peak 1	100	2405.04	1.56 min	599.02

Figure S17. (A) GC/MS and SFC of 30% methanol co-solvent data. (B) GC/MS and SFC of 30% DMSO co-solvent data. (C) SFC of ethyl R,R-2-phenylcyclopropane-1-carboxylate standard. SFC detection using a IC Daicel 5uM 4.6 x 250 mm analytical chiral column, with 10% isopropanol, and detection at max absorbance (220 nm).

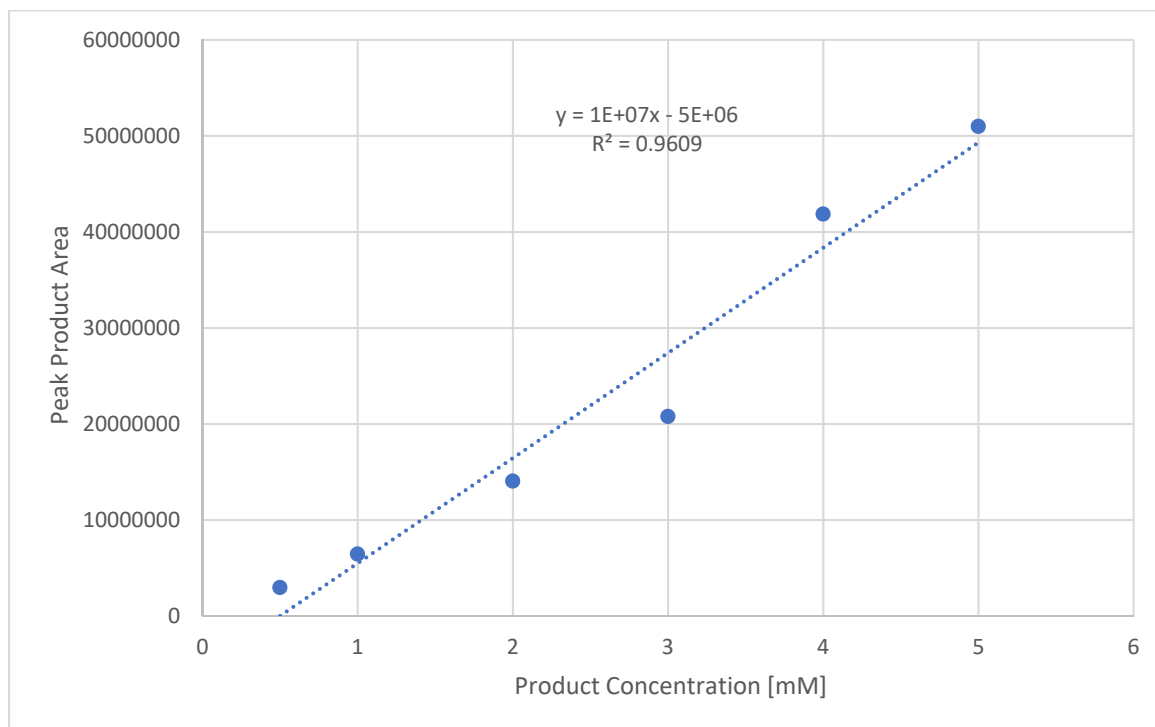
Calibration Curves

Ethylphenylglycinate



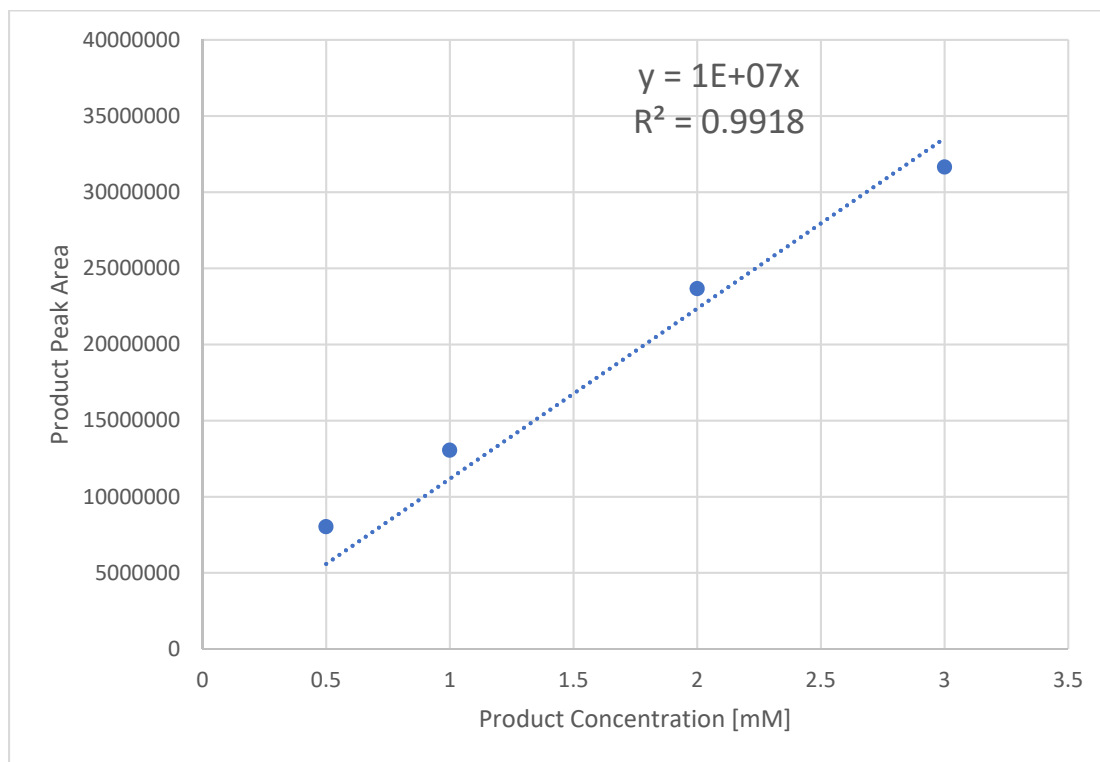
Calibration curve for the N-H insertion of aniline and ethyl diazoacetate.

Ethyl 2-phenylcyclopropanecarboxylate



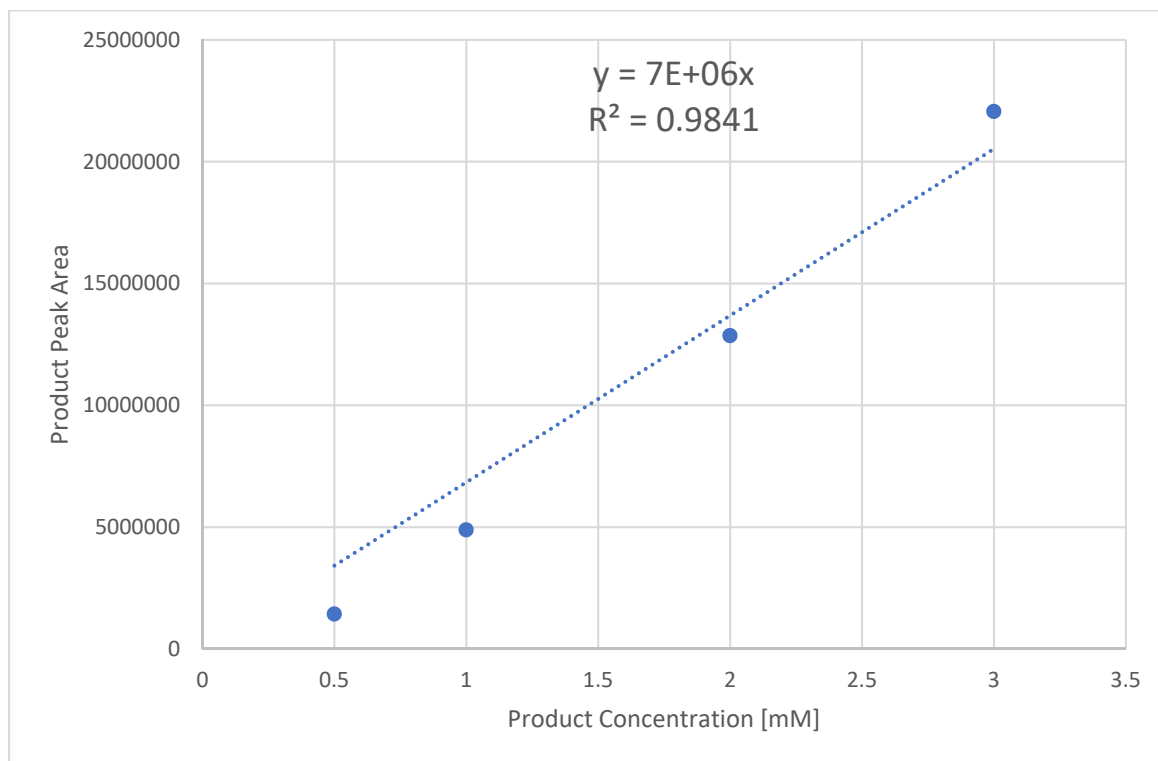
Calibration curve for the cyclopropanation of styrene and ethyl diazoacetate.

Ethyl (4-(trifluoromethyl)phenyl)glycinate



Calibration curve for the N-H insertion of benzylamine and ethyl diazoacetate.

Ethyl (4-nitrophenyl)glycinate



Calibration curve for the N-H insertion of 4-nitroaniline and ethyl diazoacetate.

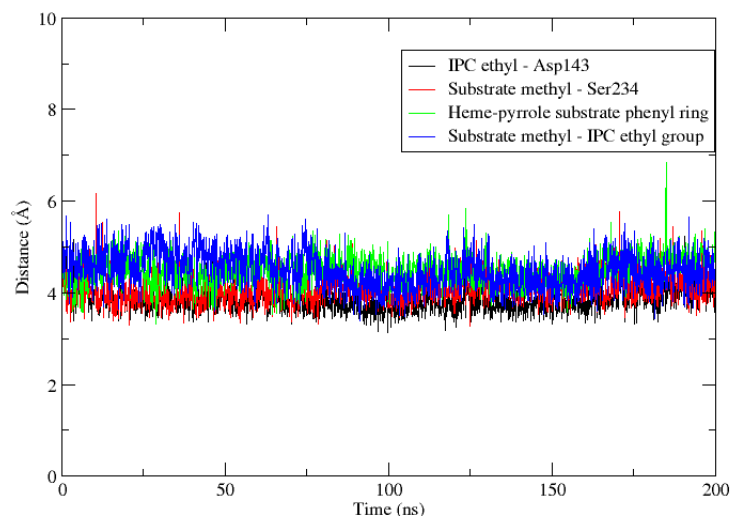


Figure S18. Dynamics of the hydrophobic interactions between the ethyl group of IPC, the substrate methyl group and the methylene groups of the Asp143 and Ser234 side chains, and of the π -stacking interaction between one of the heme pyrroles with the phenyl ring of the substrate.

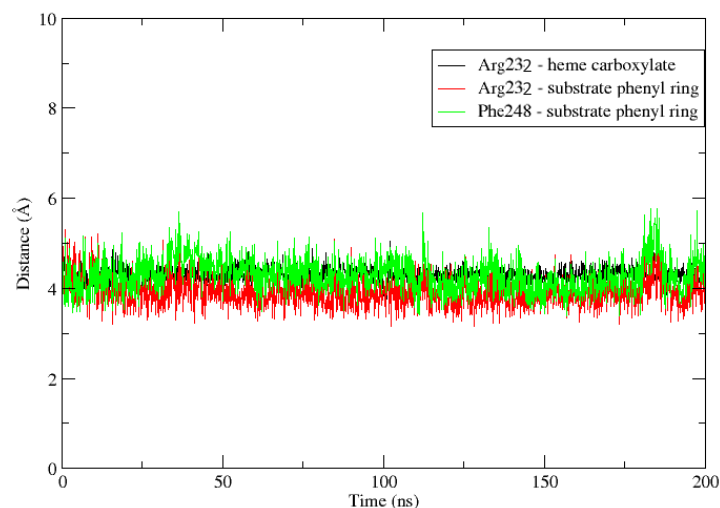


Figure S19. Dynamics of the π - π stacking and cation- π stacking interactions of the Phe248 and Arg232 side chains with the phenyl ring of the substrate, and of the salt bridge between the guanidinium group of Arg232 and one of the heme carboxylates.

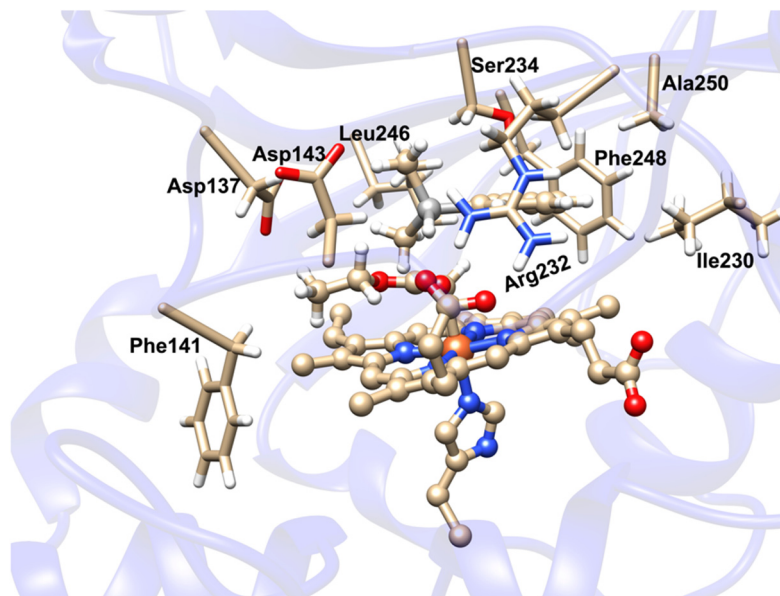


Figure S20. Second coordination sphere (SCS) residues that stabilize the open-shell singlet (OSS) transition state. The Yfex-IPC center and the dimethylphenylsilane substrate are represented in ball and stick while the SCS residues are in stick representation.

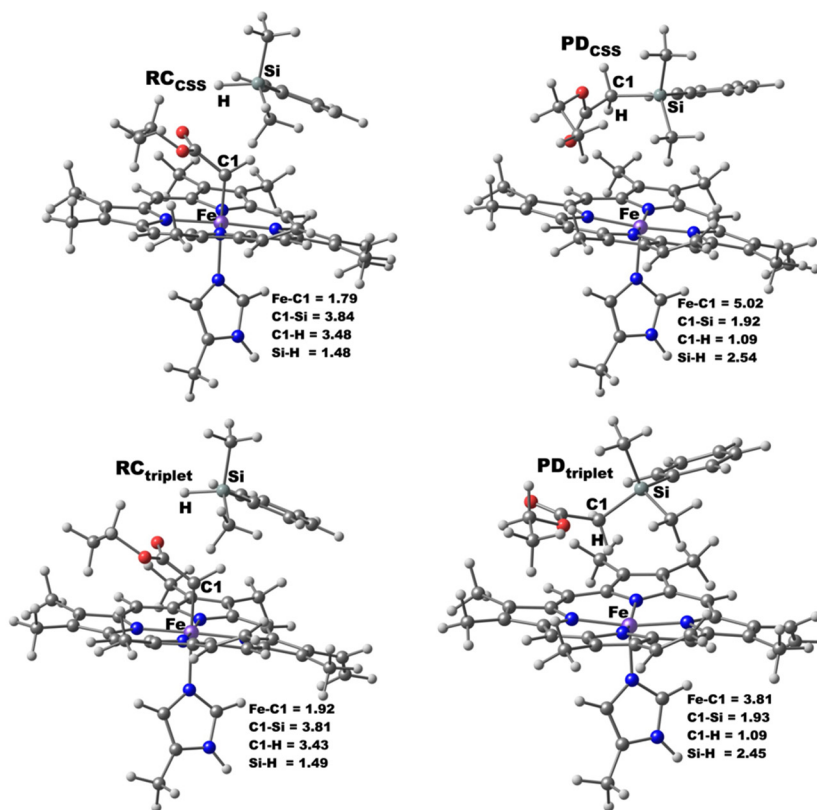


Figure S21. Stationary point geometries involved in the Si-H insertion reaction in Yfex. The distances are in Å.

The Cartesian coordinates of the optimized QM regions of the QM/MM geometries, calculated at the BS2+ZPE level of theory.

RC_{triplet}

QM/MM Energy = -2762.388526 a.u.

6	52.127525618	31.861138887	43.881388324
1	52.301189478	32.562063665	44.707777657
1	51.883967894	30.885753211	44.310121460
6	50.968504192	32.292454461	43.045211095
7	50.925086479	33.401143061	42.223761144
1	51.697107433	34.062302074	42.026858296
6	49.676517203	33.518833578	41.736958743
1	49.396585597	34.302744304	41.053019162
7	48.892427817	32.543538995	42.204857594
6	49.702301803	31.765538466	43.011365019
1	49.334963616	30.888265480	43.518191149
6	46.421423487	30.118312329	39.820150268
6	46.901806609	30.027579439	44.629522719
6	46.795548934	34.855780673	44.709618199
6	46.747894771	34.935368423	39.879240157
6	46.613224426	29.676431884	41.142571785
6	46.577500014	28.275481082	41.529304177
6	46.796819843	28.242288307	42.879911357
6	46.893654644	29.632387287	43.315293077
6	46.850247435	27.040235298	43.767827574
6	46.295675372	27.125872423	40.611240552
6	46.770977652	31.356201110	45.084707574
6	46.584591212	31.723971524	46.477695518
6	46.510537925	33.099666199	46.508410326
6	46.666063648	33.552626869	45.125829017
6	46.392256660	30.764778905	47.611830828
6	46.343381580	33.905170981	47.713147946
6	45.821319865	35.137772175	47.835736560
6	46.929839747	35.286425674	43.372914589
6	47.149734506	36.666452612	43.001483274
6	47.203269246	36.691721260	41.624500592
6	46.951746854	35.319560562	41.180214915
6	47.363270782	37.801727997	43.957568575
6	47.467532945	37.851083508	40.777218494
6	48.261134996	37.863452100	39.693081030
6	46.528800446	33.605517257	39.453239290
6	46.270045672	33.229697845	38.064618656
6	46.205961905	31.863152406	38.042857560
6	46.412324813	31.425095706	39.417549730
6	46.161927220	34.196098271	36.928526248
6	45.981892827	30.956301360	36.874341275
7	46.810380243	30.487800421	42.217881398
7	46.788774740	32.452607818	44.285895710
7	46.837650397	34.478985220	42.280141906
7	46.610811796	32.520902417	40.255102935
1	46.236839398	29.361444995	39.069174513
1	46.931224202	29.247045023	45.380137178
1	46.827792413	35.625952449	45.468843959
1	46.762720095	35.708311230	39.120903336
1	46.893401650	26.252812979	40.889418729
1	46.536735681	27.363801558	39.574570674
1	46.683171811	33.410460750	48.622509557
1	47.027207610	38.788182188	41.116204831
1	45.315994217	30.126383520	37.131012937
1	45.513614011	31.518700320	36.067598245
1	45.397048360	35.684916997	47.000248669
1	45.787840530	35.627719160	48.804275518
1	48.813152958	36.994193678	39.346546330

1	48.432033577	38.791251045	39.155655395
1	46.026078667	27.027300587	44.491326662
1	46.768789186	26.123758137	43.182621456
1	47.788392834	26.995351553	44.329157357
1	46.750485887	31.175768279	48.559916292
1	45.329653197	30.533562839	47.748621639
1	46.910821789	29.817167378	47.452729423
1	47.401394981	38.758901297	43.434664134
1	48.311310239	37.694195476	44.498291683
1	46.561898726	37.870136899	44.702235256
1	45.758354456	33.715053688	36.036707830
1	47.145585036	34.598533076	36.658427316
1	45.511854941	35.040537517	37.182538312
26	46.792957309	32.480085838	42.241913125
6	44.945798742	32.486604117	42.419745775
1	44.382739401	33.395047277	42.189531224
6	44.112377648	31.319525030	42.672686727
8	43.725131722	30.956822441	41.567902836
8	43.926096948	30.814158233	43.855511789
6	43.148036389	29.555806952	43.977411991
6	43.269039090	29.111912940	45.419034378
1	42.124432230	29.791644180	43.681230770
1	43.567917459	28.840992842	43.268844284
1	42.783351173	29.814691072	46.101803122
1	44.321715024	29.018043225	45.699699079
1	42.805469713	28.130812357	45.547345472
6	42.737010259	36.412230850	40.628110755
6	42.370620473	35.724279402	41.789461989
6	41.945043927	34.382143788	41.745651595
6	41.907760204	33.752749634	40.484527319
6	42.265095523	34.433133456	39.317874104
6	42.676869629	35.766843764	39.388157992
1	43.087132342	37.437565328	40.689990329
1	42.428983934	36.241437015	42.744359954
1	41.611736403	32.709568797	40.419695232
1	42.239335931	33.920243600	38.360002253
1	42.963025762	36.297630992	38.485139337
14	41.353303433	33.433976858	43.278096668
1	41.595589760	32.001493913	42.972533230
6	42.328991115	33.911966093	44.830713030
1	41.724457692	33.719734943	45.723271724
1	42.603028358	34.970970580	44.843626119
1	43.249509428	33.326054524	44.922209745
6	39.510368779	33.621620009	43.492036018
1	39.210223079	34.610088762	43.850663038
1	39.168899437	32.877016327	44.214928834
1	39.010086889	33.408560501	42.546228927
1	53.090814016	31.761078814	43.381257582
1	45.254646122	26.805659236	40.653536356
1	46.911044948	30.533593012	36.492161587

TS_{triplet}

QM/MM Energy = -2762.344452 a.u.

6	52.036939934	31.760588955	43.883399938
1	52.193692830	32.414332861	44.750820448
1	51.803047601	30.759216956	44.252627151
6	50.874850032	32.230800681	43.068904922
7	50.843743522	33.365633473	42.281389346
1	51.630558176	34.012003475	42.088092988
6	49.589349115	33.540541382	41.831688931
1	49.318829372	34.350085834	41.174856339
7	48.789953595	32.572272161	42.292256218
6	49.593577818	31.739137278	43.051459863
1	49.206076353	30.861752541	43.542518067
6	46.430618561	30.137571846	39.890266258

6	46.668476357	30.087336960	44.702162139
6	46.827802774	34.925302191	44.755374065
6	46.722728159	34.966742644	39.934889924
6	46.567182391	29.697252940	41.221428969
6	46.474517856	28.295060222	41.613463653
6	46.583935884	28.272544180	42.974028786
6	46.697605877	29.668613206	43.395992374
6	46.499518899	27.083944429	43.878579467
6	46.239392911	27.140908354	40.687905778
6	46.625125078	31.429703517	45.136196494
6	46.502340620	31.812185223	46.531158687
6	46.498905932	33.189268862	46.555011389
6	46.646283426	33.626462590	45.167914727
6	46.323174513	30.865993272	47.678614865
6	46.396362541	34.011265151	47.756958297
6	45.884958933	35.247184890	47.886679364
6	46.941885075	35.353397897	43.417331913
6	47.191649281	36.728472381	43.034302550
6	47.224065780	36.742958206	41.658887059
6	46.928750383	35.370937852	41.230307971
6	47.444047090	37.861529916	43.983223103
6	47.513739279	37.888780804	40.799709591
6	48.286888084	37.871880131	39.700978742
6	46.500383622	33.631971828	39.525147498
6	46.263133840	33.250400899	38.138487699
6	46.208517112	31.880955342	38.117147716
6	46.402067543	31.445602431	39.493147139
6	46.163297979	34.213676602	36.998674799
6	45.981378404	30.975904033	36.945405891
7	46.719848123	30.512937647	42.292335954
7	46.686902785	32.520109408	44.327853766
7	46.798421239	34.543958269	42.335282202
7	46.564285067	32.547049494	40.337899484
1	46.281421978	29.380453100	39.131753813
1	46.629013493	29.320159269	45.466060381
1	46.909729371	35.688769302	45.518226917
1	46.754015923	35.723792602	39.160983453
1	46.829371525	26.273372801	41.001540842
1	46.526175155	27.371671080	39.660980482
1	46.775094905	33.526479190	48.656332715
1	47.115347764	38.844636711	41.139854508
1	45.318344103	30.145025980	37.206295476
1	45.505555906	31.537943951	36.142082171
1	45.431471387	35.785846942	47.060694015
1	45.894684253	35.749126730	48.849705141
1	48.802787683	36.984294010	39.345049716
1	48.477208412	38.793177367	39.159211382
1	45.474967154	26.924277460	44.237881881
1	46.788731416	26.174371226	43.347834943
1	47.147686648	27.180290810	44.752944311
1	46.669352654	31.300719002	48.620209816
1	45.267589199	30.608984503	47.817940138
1	46.866312918	29.929106924	47.536534700
1	47.509372302	38.813939816	43.454490824
1	48.389969203	37.728589770	44.522056356
1	46.647030724	37.957560606	44.729832489
1	45.851093891	33.713157905	36.081362601
1	47.134867112	34.678965075	36.794618331
1	45.444623807	35.011830413	37.214092511
26	46.762202030	32.526051090	42.311808788
6	44.404909430	32.426962618	42.258755403
1	43.972427385	32.904677930	41.392238284
6	43.726367843	31.338350051	42.875192546
8	43.845313654	30.511215302	41.963527966
8	43.286388849	31.215635598	44.089354464
6	42.606495972	29.942887436	44.439302125

6	42.755114624	29.743705172	45.930102774
1	41.566789172	30.074435777	44.130089920
1	43.057706605	29.142470778	43.849777936
1	42.355232724	30.594592724	46.487870348
1	43.806748852	29.611677671	46.196180604
1	42.212382484	28.845482329	46.236667717
6	41.983402276	36.516584805	39.134231030
6	41.967015525	36.018998263	40.440343035
6	42.075354882	34.637234687	40.698295073
6	42.269565743	33.787302347	39.592998108
6	42.349919488	34.282694444	38.287227565
6	42.179015244	35.647255463	38.055825487
1	41.851236374	37.577766676	38.955565952
1	41.865508993	36.722867304	41.266885856
1	42.361997466	32.715980964	39.754157541
1	42.518115735	33.601446852	37.457256882
1	42.203794260	36.037529505	37.042663287
14	41.954784519	33.884314444	42.429774949
1	42.267754925	32.413967469	42.150560013
6	43.254565706	34.616579269	43.596752639
1	43.101956571	34.241564682	44.613049495
1	43.116940971	35.704546796	43.608123510
1	44.301891960	34.446381959	43.322072822
6	40.275019437	33.980557101	43.264886155
1	39.995837146	34.990961970	43.580477094
1	40.308590759	33.370949911	44.173818466
1	39.484139855	33.563094122	42.634870662
1	53.006592900	31.704498447	43.388734095
1	45.201028242	26.809483341	40.683047338
1	46.905569239	30.553313803	36.551253482

PD_{triplet}
QM/MM Energy = -2762.503464 a.u.

6	52.117705178	31.802580656	43.898471335
1	52.294166079	32.468641952	44.752098104
1	51.861352658	30.813899995	44.285361114
6	50.969812852	32.285155376	43.075511954
7	50.979074364	33.388024582	42.236704883
1	51.784429696	34.009312217	42.032455568
6	49.745419028	33.584028903	41.760804321
1	49.497124020	34.374389320	41.071907768
7	48.915557149	32.653463731	42.258155612
6	49.678882704	31.829489219	43.069376000
1	49.255863418	30.985332024	43.588742430
6	46.524026293	30.278885783	39.902176001
6	46.581496049	30.328291348	44.720437000
6	46.918238065	35.144659877	44.628904878
6	46.854936845	35.097366322	39.816886429
6	46.548038309	29.870246645	41.229064786
6	46.357631524	28.482202259	41.655830224
6	46.409982130	28.493815085	43.019651781
6	46.583742993	29.888475722	43.408399094
6	46.222643461	27.341377338	43.955671712
6	46.076570173	27.304374683	40.775450719
6	46.590677142	31.662173268	45.105375898
6	46.482245633	32.096918599	46.490373113
6	46.505154023	33.467333683	46.464220427
6	46.685855200	33.852809575	45.058048249
6	46.294665533	31.196180783	47.671639441
6	46.404779788	34.339006746	47.631499997
6	45.881896356	35.573964292	47.707287165
6	47.062900509	35.531721618	43.298932027
6	47.314089159	36.904239044	42.890034635
6	47.366137049	36.895175952	41.521076814
6	47.076139778	35.511958350	41.112703752

6	47.531842290	38.052601321	43.825961505
6	47.648470140	38.032047225	40.646300249
6	48.456909739	38.009342536	39.574447715
6	46.585544630	33.776757993	39.452737021
6	46.337220401	33.357701170	38.078581474
6	46.295179692	31.992013432	38.092504440
6	46.497189503	31.592972971	39.487126462
6	46.205713922	34.297512577	36.924701259
6	46.048872797	31.053888889	36.951761786
7	46.674363100	30.716193449	42.303797473
7	46.693490037	32.736791256	44.246854758
7	46.940740222	34.693154932	42.218811300
7	46.628027165	32.698721049	40.312879037
1	46.411850311	29.513265975	39.147298543
1	46.507660101	29.579638301	45.498869931
1	47.002064679	35.918465481	45.380070104
1	46.900836759	35.841131000	39.031268954
1	46.559854059	26.415149642	41.193798106
1	46.457896521	27.429358369	39.760218388
1	46.781199790	33.893225000	48.551039201
1	47.217047037	38.983234070	40.956066952
1	45.376938788	30.241432914	37.246320464
1	45.571876415	31.597579274	36.136392187
1	45.427548565	36.074413345	46.858268741
1	45.878447089	36.109697640	48.651571982
1	48.991147706	37.122581789	39.243155192
1	48.654089612	38.927798853	39.030950866
1	45.168039417	27.215179095	44.231676532
1	46.536820027	26.406064594	43.487294696
1	46.795549018	27.457922463	44.879469501
1	46.651013027	31.665551393	48.592654779
1	45.237241117	30.956884910	47.823079037
1	46.826087557	30.247846468	47.561808147
1	47.683543908	38.983003253	43.277704717
1	48.420907414	37.896634752	44.448642183
1	46.678470113	38.202484914	44.497515009
1	45.904198256	33.772902725	36.017861437
1	47.162395050	34.787537149	36.709836018
1	45.462789198	35.073888077	37.134832962
26	46.991403853	32.691623920	42.253027065
6	43.294982667	31.829639479	41.915905321
1	43.420025457	31.494843723	40.885372936
6	42.841601602	30.643933030	42.718891119
8	42.481872592	29.578966987	42.259923149
8	42.875693878	30.905255795	44.050324641
6	42.317331932	29.877343499	44.909187804
6	42.747579929	30.151464490	46.332024939
1	41.227836036	29.912937771	44.806908283
1	42.661240967	28.901376348	44.560431268
1	42.472593617	31.163126271	46.641117476
1	43.830209168	30.039533013	46.435657005
1	42.266083714	29.434609391	47.002989548
6	41.863606321	36.299464385	39.031125801
6	41.942604605	35.651699033	40.267586216
6	42.222533093	34.272486737	40.366497556
6	42.477026752	33.588477083	39.164447141
6	42.430054248	34.231100165	37.922637749
6	42.102358977	35.585532091	37.852994144
1	41.637585933	37.360843147	38.984990149
1	41.805494801	36.238822149	41.176017952
1	42.727326172	32.533058465	39.185490747
1	42.629270676	33.666893705	37.015656763
1	42.042462521	36.086602630	36.891057895
14	42.192091082	33.400664203	42.055574279
1	44.276310029	32.142464790	42.290545335
6	42.958463688	34.544760629	43.354890669

1	42.925231626	34.062139685	44.337855327
1	42.408455704	35.488012133	43.434267368
1	44.002179439	34.783126854	43.122154504
6	40.436595968	32.973886265	42.586721729
1	39.915794520	33.859293610	42.966842252
1	40.448043490	32.250199504	43.408256814
1	39.838399792	32.545405626	41.780448339
1	53.081060273	31.713921257	43.396322163
1	45.012358709	27.072900351	40.731394967
1	46.964481076	30.609673540	36.561375399

RC_{oss}
QM/MM Energy = -2762.385180 a.u.

6	52.126033846	31.860573355	43.882024665
1	52.299015501	32.560831476	44.709112491
1	51.882469492	30.884707493	44.309660256
6	50.966985998	32.292809587	43.046218246
7	50.923793651	33.401759415	42.225089649
1	51.695908640	34.063021898	42.028396852
6	49.675465595	33.520261103	41.738242775
1	49.395892142	34.304731862	41.054742348
7	48.891105001	32.544652014	42.205964829
6	49.700612701	31.766190042	43.012376287
1	49.333526778	30.888440786	43.518476868
6	46.422481413	30.120164798	39.819748770
6	46.900498784	30.029919942	44.629030939
6	46.789499258	34.858425316	44.708441351
6	46.749522822	34.937185369	39.878282770
6	46.614177977	29.677629550	41.143359169
6	46.578543091	28.276576966	41.530368627
6	46.797908302	28.243849253	42.881369235
6	46.893469337	29.633137983	43.315900361
6	46.853416085	27.041844653	43.769592645
6	46.296334542	27.126829757	40.612561093
6	46.768088905	31.358853727	45.085224787
6	46.581380540	31.725262378	46.477042498
6	46.504583676	33.101790184	46.507670615
6	46.659951090	33.554722596	45.125630179
6	46.390183005	30.766165016	47.611740921
6	46.336190950	33.906691656	47.712385317
6	45.814941210	35.139798120	47.834717386
6	46.926451769	35.288297533	43.372293986
6	47.148374007	36.668441615	42.999496600
6	47.203782823	36.693331795	41.623029696
6	46.952900900	35.322767556	41.178907186
6	47.359533589	37.803433827	43.956090106
6	47.469895139	37.852621810	40.775045316
6	48.265669473	37.863095926	39.692948212
6	46.530360365	33.606935579	39.452128812
6	46.271284365	33.231085602	38.063878771
6	46.206977502	31.864316945	38.042425100
6	46.413730980	31.426384290	39.417165838
6	46.162833505	34.197230218	36.927635097
6	45.983214262	30.957345162	36.873888945
7	46.809813356	30.488335827	42.216673281
7	46.784381219	32.455781024	44.286416177
7	46.836307854	34.481099452	42.279921038
7	46.612557303	32.522942359	40.254430647
1	46.237438707	29.363159313	39.068964673
1	46.931815806	29.249905406	45.380068628
1	46.820698702	35.628978633	45.467433882
1	46.765479458	35.709919707	39.119583636
1	46.894264235	26.253813669	40.890584586
1	46.536862763	27.364867903	39.575759873
1	46.673907595	33.411037432	48.622113060

1	47.027325722	38.789570685	41.111307666	6	49.596398031	33.548076284	41.825026976
1	45.316943661	30.127431360	37.129861633	1	49.323503213	34.357467592	41.168789634
1	45.515619592	31.519839310	36.066810936	7	48.798634330	32.577353649	42.283044020
1	45.392170647	35.687847496	46.998982200	6	49.602147627	31.745627225	43.044014689
1	45.780438827	35.629168693	48.803534479	1	49.216638329	30.866706661	43.533696164
1	48.817205043	36.992588504	39.348820845	6	46.418726757	30.144038498	39.878722934
1	48.438081364	38.789750219	39.154174535	6	46.696681251	30.085276740	44.687632022
1	46.035372105	27.032794521	44.499989183	6	46.820555580	34.923780696	44.744660761
1	46.763588665	26.125335746	43.185722509	6	46.731232525	34.971023735	39.925040305
1	47.796072021	26.993478429	44.323115386	6	46.563196740	29.700065136	41.209508485
1	46.746491631	31.178791362	48.559830459	6	46.477047287	28.298282790	41.600514231
1	45.328047245	30.532600154	47.747707575	6	46.606127435	28.273432923	42.959955073
1	46.911312696	29.819581082	47.454470019	6	46.720326139	29.666721910	43.382603851
1	47.400154531	38.760496999	43.433168780	6	46.543617208	27.082111184	43.862318331
1	48.305533872	37.694542982	44.500247490	6	46.229924051	27.145699567	40.676017065
1	46.555322640	37.871890159	44.697771254	6	46.640129994	31.427848143	45.125666163
1	45.758572048	33.716053859	36.036221771	6	46.508052380	31.806928451	46.518026958
1	47.146575725	34.599085108	36.657108686	6	46.492032925	33.185901485	46.542602659
1	45.513113922	35.041846035	37.181855827	6	46.641028235	33.623691125	45.158534870
26	46.794267812	32.483529623	42.240274036	6	46.329362621	30.860129375	47.665536657
6	44.947333133	32.484568673	42.423271990	6	46.379940081	34.005319945	47.745209938
1	44.384987436	33.393790825	42.194728575	6	45.866279336	35.240472895	47.873861405
6	44.112807346	31.317804458	42.673270526	6	46.940018704	35.354626265	43.408725967
8	43.724545071	30.955987060	41.568717282	6	47.191399874	36.729098329	43.027637542
8	43.926517343	30.812113323	43.855968887	6	47.226507388	36.745206786	41.651593160
6	43.148741274	29.553906364	43.977347193	6	46.934350099	35.376108793	41.221784291
6	43.269022199	29.111161138	45.419318461	6	47.441750212	37.861504013	43.978239217
1	42.125245915	29.789102452	43.680038740	6	47.516668772	37.893355726	40.793881079
1	43.569685043	28.838976169	43.269477673	6	48.296466938	37.879502162	39.700453914
1	42.782531779	29.814332179	46.101120118	6	46.505081552	33.637590579	39.512871787
1	44.321608697	29.018373971	45.700854993	6	46.264668845	33.257474375	38.127104636
1	42.806062212	28.129855832	45.547870056	6	46.205680854	31.887166470	38.106061506
6	42.737629311	36.410879570	40.629795883	6	46.397975802	31.451767018	39.479761368
6	42.370818105	35.722950591	41.791020332	6	46.164507139	34.220849277	36.987098903
6	41.945230033	34.380825153	41.747211726	6	45.978656025	30.982121315	36.934290078
6	41.908092717	33.751357374	40.486093890	7	46.725359387	30.514072886	42.277623869
6	42.265829190	34.431688379	39.319537631	7	46.693567339	32.518710988	44.317782565
6	42.677944246	35.765318204	39.389897467	7	46.800268957	34.546050890	42.325261161
1	43.087726677	37.436251519	40.691663101	7	46.567803386	32.552964505	40.324924190
1	42.428986575	36.240093539	42.745921318	1	46.262781487	29.387282196	39.120906902
1	41.612043452	32.708167011	40.421284536	1	46.670712264	29.317766012	45.452135992
1	42.240055591	33.918840846	38.361634247	1	46.898482936	35.686950281	45.508557367
1	42.964869246	36.295935371	38.487028574	1	46.766134474	35.729199629	39.152052428
14	41.353017529	33.432512995	43.279408382	1	46.826569368	26.277870977	40.975236261
1	41.596073523	32.000259437	42.973478346	1	46.499264502	27.381214506	39.645511557
6	42.327728064	33.910709340	44.832598923	1	46.754627657	33.519191318	48.645733543
1	41.722671227	33.719504307	45.725027598	1	47.109193538	38.847067370	41.129680932
1	42.602493296	34.969549294	44.844871199	1	45.312751350	30.152757122	37.193072279
1	43.247785977	33.324190539	44.924828733	1	45.507326088	31.546027927	36.129925255
6	39.509900484	33.619820881	43.491870571	1	45.414563555	35.778443186	47.046460544
1	39.209290663	34.608198234	43.850324921	1	45.871572225	35.742367686	48.836971856
1	39.167597433	32.875108749	44.214209100	1	48.818878307	36.993800028	39.349229571
1	39.010578224	33.406890169	42.545569086	1	48.484706589	38.800878838	39.157983166
1	53.089538169	31.761075766	43.382197718	1	45.553160829	26.972207245	44.321665118
1	45.255324982	26.806587990	40.655124332	1	46.729957710	26.164564381	43.301184910
1	46.912401976	30.534508912	36.491937353	1	47.280369726	27.134596434	44.668191193

TS_{oss}

QM/MM Energy = -2762.358976 a.u.

6	52.043597069	31.772483483	43.881172737	26	46.771043984	32.529173812	42.297610613
1	52.201992313	32.430985466	44.744638191	1	48.385440182	37.727218730	44.520641912
1	51.808012877	30.773610789	44.256480138	1	46.642567919	37.958260125	44.722444312
6	50.882089923	32.240727427	43.064895510	1	45.842052543	33.722044453	36.072391792
7	50.849677451	33.375472508	42.277618217	1	47.137311223	34.680164059	36.775092072
1	51.635269277	34.023096538	42.084877088	1	45.452490816	35.023820750	37.206637870

6	44.405830627	32.445952456	42.249941776	6	46.380799126	34.288584764	47.631999916
1	43.960893136	32.973772291	41.420994548	6	45.856038830	35.522404770	47.708354944
6	43.732591100	31.360825182	42.862094748	6	47.040116449	35.490301353	43.299095342
8	43.849906034	30.585317622	41.900765211	6	47.279971218	36.863699987	42.890738419
8	43.313849920	31.181821865	44.072292863	6	47.331743412	36.855714570	41.520928460
6	42.654686196	29.886213806	44.385845147	6	47.049586669	35.471151439	41.111512558
6	42.874726632	29.610101479	45.855213917	6	47.484958937	38.014637585	43.826437060
1	41.601818367	30.034167410	44.135517072	6	47.604374276	37.995066673	40.647835387
1	43.078180182	29.121964635	43.731047638	6	48.402021665	37.979391972	39.567553678
1	42.487871027	30.423227049	46.475635590	6	46.568147780	33.735121677	39.452509909
1	43.939493822	29.480758071	46.064915816	6	46.317617278	33.314570065	38.079350967
1	42.357842642	28.688851806	46.136789147	6	46.288427755	31.947936809	38.092868053
6	41.990635044	36.506157081	39.152742417	6	46.499474078	31.550051219	39.485356026
6	41.969668465	36.013591500	40.460450516	6	46.173402317	34.252714505	36.925589552
6	42.065936284	34.632086194	40.723655242	6	46.044089538	31.009204390	36.952192324
6	42.250592913	33.775476257	39.621481893	7	46.682690154	30.675516514	42.303053809
6	42.336457790	34.265778653	38.313948471	7	46.691244939	32.692440557	44.246388617
6	42.179188783	35.631363455	38.077483976	7	46.921701943	34.651942338	42.216657924
1	41.867163471	37.567633535	38.970264057	7	46.625005034	32.657138687	40.310971543
1	41.874167132	36.720877847	41.284515481	1	46.419400479	29.470198223	39.146228457
1	42.333590480	32.703896530	39.787052570	1	46.519170812	29.533429258	45.496070054
1	42.499078843	33.580721434	37.485678060	1	46.977266851	35.876410887	45.380146052
1	42.207738377	36.017570241	37.062834683	1	46.866695772	35.801109652	39.029807774
14	41.941837398	33.890095520	42.459330260	1	46.531241588	26.372725089	41.192972188
1	42.265187611	32.419015921	42.188324954	1	46.440246803	27.387109662	39.758817032
6	43.219752490	34.647507562	43.630270858	1	46.750658140	33.839146213	48.552630574
1	43.075830164	34.266099922	44.645909243	1	47.173901628	38.944317851	40.964597644
1	43.050867232	35.730769232	43.648558716	1	45.387024383	30.186075973	37.250461631
1	44.270153321	34.505568370	43.353776217	1	45.551554384	31.547713896	36.142553382
6	40.252760146	33.975484582	43.278831584	1	45.406776606	36.024931520	46.857814273
1	39.968105491	34.981986542	43.601561077	1	45.845019518	36.055177355	48.654325789
1	40.277690316	33.358521225	44.183363818	1	48.937245791	37.096746028	39.226950700
1	39.468898402	33.561213844	42.637794398	1	48.588467548	38.901506766	39.026509217
1	53.012836864	31.711544876	43.386270700	1	45.171923012	27.194781873	44.245209790
1	45.191572221	26.814366837	40.686572701	1	46.515895665	26.363747592	43.479697018
1	46.902810781	30.556525088	36.543300107	1	46.812125940	27.408514744	44.869876825

PD_{oss}

QM/MM Energy = -2762.508344 a.u.

6	52.105268057	31.800858507	43.905616344	1	46.632846784	38.147962718	44.502966429
1	52.281868963	32.469315081	44.757452060	1	45.864492362	33.726360110	36.022166463
1	51.851691977	30.812337155	44.294978984	1	47.126936925	34.744621986	36.700581354
6	50.954223365	32.278130379	43.083596702	1	45.430957366	35.027834115	37.141367624
7	50.954679140	33.384280875	42.248262506	26	46.984302241	32.651527906	42.250964792
1	51.756545288	34.012263846	42.046749323	6	43.374260912	31.997596443	42.065684068
6	49.720666482	33.571441671	41.771774462	1	43.602217548	31.695302981	41.042822842
1	49.465297876	34.363060874	41.086427127	6	42.889391568	30.777851345	42.795777768
7	48.898181026	32.631253924	42.265572714	8	42.526090807	29.743451405	42.274229313
6	49.667717863	31.810362128	43.074775434	8	42.898414019	30.969039942	44.138565122
1	49.252377378	30.960926856	43.591823401	6	42.320925120	29.895818723	44.926189444
6	46.530989763	30.236472618	39.900352245	6	42.717756256	30.089811350	46.371277021
6	46.590333600	30.283830976	44.719280880	1	41.234299629	29.935862163	44.799054689
6	46.898837517	35.102022103	44.629154147	1	42.674934153	28.940816706	44.531717910
6	46.828685352	35.057166251	39.815537604	1	42.435078818	31.081862987	46.731086355
6	46.554065172	29.829827277	41.227157229	1	43.798258039	29.976173632	46.492783626
6	46.359903515	28.443101674	41.653880645	1	42.222029406	29.335293098	46.988552323
6	46.416947822	28.453613823	43.017350230	6	41.845876539	36.267756497	38.948057864
6	46.593290314	29.847947878	43.406426406	6	41.931301537	35.683769296	40.215583148
6	46.224381687	27.303115828	43.954107411	6	42.221903346	34.314119736	40.385030444
6	46.060484502	27.268580864	40.775242250	6	42.485537128	33.572434492	39.219619129
6	46.590338500	31.616877050	45.103750700	6	42.437480277	34.151818025	37.947224076
6	46.473977826	32.050105458	46.488158802	6	42.095318322	35.497730208	37.808550500
6	46.491586474	33.420797397	46.462913978	1	41.608937330	37.323225841	38.849460172
6	46.675213609	33.808656724	45.057938772	1	41.794987298	36.316260847	41.093101841
6	46.283975570	31.147386735	47.667366859				

1	42.744534334	32.521391668	39.295333529
1	42.646359868	33.547036154	37.069014716
1	42.031385153	35.947953841	36.822025246
14	42.207519382	33.529899220	42.116987056
1	44.300960058	32.339892254	42.541300895
6	42.922427754	34.774617282	43.351195377
1	42.858351957	34.379386135	44.371126617
1	42.363193280	35.714843913	43.330086534
1	43.971140378	35.006056883	43.135321350
6	40.472162992	33.053930569	42.671693953
1	39.895239609	33.935609071	42.969142712
1	40.519192435	32.411707121	43.557285161
1	39.907109256	32.519712091	41.905646183
1	53.068010747	31.712089955	43.402313275
1	44.992167449	27.055823241	40.736509962
1	46.962550728	30.578734467	36.553203595

RC_{css}

QM/MM Energy = -2762.381195 a.u.

6	52.136059627	31.842598881	43.888858549
1	52.309701537	32.537025570	44.720968331
1	51.893646747	30.863692029	44.310100436
6	50.977804963	32.278664578	43.055017146
7	50.937884329	33.384722611	42.231762262
1	51.709419847	34.046639581	42.038080007
6	49.687298946	33.499685236	41.743771217
1	49.413943775	34.281582056	41.055070634
7	48.897837500	32.528185055	42.210479372
6	49.708396983	31.754893235	43.017371741
1	49.344117858	30.875017665	43.522788053
6	46.404237778	30.141464072	39.820299681
6	46.908053409	29.992287846	44.613967141
6	46.819609025	34.824514579	44.720594875
6	46.794582407	34.958959944	39.902695468
6	46.592344214	29.672677324	41.164187258
6	46.566655479	28.242572554	41.528287389
6	46.788066166	28.190224034	42.869015291
6	46.879520087	29.586737245	43.319017215
6	46.835564735	26.983963949	43.750258577
6	46.299044580	27.111409109	40.586032617
6	46.793963413	31.349898577	45.073800733
6	46.598167863	31.706482401	46.486804537
6	46.539899648	33.074166619	46.528442378
6	46.705340422	33.535124575	45.136057172
6	46.381626971	30.732523721	47.601891398
6	46.376068557	33.878669779	47.734014124
6	45.849715220	35.109266032	47.855601424
6	46.951175518	35.286596646	43.363929731
6	47.186084125	36.686162591	43.015680480
6	47.252250755	36.727896250	41.646884932
6	46.992848739	35.351081413	41.187761543
6	47.394465087	37.798831324	43.997803651
6	47.527154991	37.888420915	40.804441938
6	48.316251696	37.894515466	39.716910199
6	46.560869381	33.606204335	39.462726216
6	46.295514079	33.244980717	38.061786563
6	46.216735319	31.884335784	38.031433438
6	46.416635285	31.434616552	39.414218395
6	46.192183453	34.229612315	36.941694136
6	45.987787862	30.982426306	36.860974798
7	46.782357011	30.460910305	42.216639038
7	46.826162933	32.421068816	44.288114433
7	46.859917848	34.496754246	42.295642878
7	46.630849564	32.544450413	40.258825443
1	46.210629635	29.386239807	39.068753696

1	46.945458736	29.222589182	45.376224616
1	46.833420694	35.594534846	45.482002099
1	46.832252186	35.722887698	39.134457158
1	46.895467002	26.235482816	40.858809360
1	46.552306251	27.367365969	39.556213664
1	46.720488380	33.384954777	48.641960028
1	47.096926871	38.828201111	41.148206211
1	45.299617520	30.168327585	37.109713929
1	45.544518031	31.554949358	36.047377182
1	45.416090226	35.652112024	47.021963045
1	45.815197226	35.599897930	48.823678230
1	48.858450076	37.020675248	39.366271544
1	48.495212964	38.821163917	39.180273737
1	45.957977164	26.925173214	44.405696994
1	46.841579099	26.071407584	43.152907793
1	47.729146128	26.976288096	44.381371425
1	46.675027058	31.147975445	48.569587916
1	45.321082018	30.466721259	47.680918363
1	46.937015825	29.802692761	47.463035208
1	47.508671698	38.758581044	43.491122838
1	48.302649411	37.641878902	44.592526752
1	46.552906772	37.897411663	44.694144405
1	45.831928509	33.754406922	36.028792656
1	47.169541933	34.670374258	36.711212265
1	45.505744452	35.046485427	37.192619335
26	46.761021267	32.482026919	42.257338901
6	44.968963936	32.508617033	42.320768293
1	44.405856366	33.404956323	42.036738734
6	44.095927978	31.330419980	42.488287231
8	43.638849457	30.869152503	41.456839406
8	43.949513449	30.857943931	43.719182262
6	43.149421404	29.634278318	43.891869759
6	43.285781856	29.219249211	45.343846340
1	42.119999614	29.873810109	43.615690279
1	43.524687324	28.882005142	43.195514976
1	42.852789642	29.964420716	46.017924469
1	44.339344596	29.081882327	45.605368990
1	42.781048860	28.265663166	45.516745301
6	42.672324563	36.452414369	40.518455132
6	42.304265779	35.769387371	41.681786865
6	41.904496826	34.419302292	41.647598253
6	41.894186786	33.776774895	40.393582425
6	42.251032648	34.452825544	39.223591800
6	42.636778357	35.794638677	39.283747738
1	43.006714905	37.482843242	40.575829471
1	42.346020240	36.296451017	42.632312058
1	41.628025526	32.725238862	40.338589240
1	42.245370272	33.929467096	38.270957312
1	42.920042186	36.323395923	38.378289270
14	41.354950311	33.470486828	43.195139821
1	41.565381317	32.037842352	42.878398694
6	42.392770832	33.947934440	44.708245476
1	41.832034712	33.741467464	45.626209911
1	42.653033047	35.010849747	44.714237519
1	43.321553852	33.369863737	44.745521912
6	39.526043073	33.682783078	43.502524687
1	39.252568366	34.675389033	43.871955004
1	39.220898304	32.945095594	44.248721897
1	38.969555975	33.465281608	42.589704056
1	53.099847055	31.747971152	43.388631900
1	45.258968568	26.786326619	40.6111444083
1	46.912863286	30.539159094	36.492441268

TS_{css}**QM/MM Energy = -2762.344904 a.u.**

6	52.019624149	31.784936368	43.908108986
1	52.180735872	32.436566640	44.777167251
1	51.790769943	30.782499638	44.277922257
6	50.851410157	32.253455738	43.100819533
7	50.829780355	33.361504473	42.280893962
1	51.616397361	34.004351106	42.086392663
6	49.573531939	33.514470083	41.813377748
1	49.317978005	34.302700625	41.125417896
7	48.760018324	32.571243218	42.295157363
6	49.561848795	31.772742441	43.089142131
1	49.175752438	30.904388442	43.599695494
6	46.532903940	30.157950991	39.781111163
6	46.548363240	30.047759979	44.601151336
6	46.637075974	34.875347161	44.680013690
6	46.783438268	34.974465314	39.858776085
6	46.604039788	29.697488863	41.141393260
6	46.507448329	28.273214351	41.510375300
6	46.564006905	28.230506112	42.868137015
6	46.636200059	29.629492698	43.312415527
6	46.458315290	27.035902792	43.760996642
6	46.312137754	27.136532857	40.558841844
6	46.478151542	31.412275282	45.047811505
6	46.348738679	31.780824375	46.465896681
6	46.323722978	33.148690873	46.501881273
6	46.460565902	33.594867189	45.100900519
6	46.195512078	30.808596120	47.592336870
6	46.234438145	33.964897508	47.707420486
6	45.759919910	35.215267865	47.841025454
6	46.814464898	35.318014328	43.323759876
6	47.127878438	36.704480019	42.975290820
6	47.239722515	36.736134513	41.609615704
6	46.931844387	35.369313299	41.149106807
6	47.364516010	37.810161040	43.959117000
6	47.611469257	37.876807713	40.774990303
6	48.427790311	37.836744439	39.708178992
6	46.565450278	33.618876368	39.415248634
6	46.343003403	33.250085859	38.009346823
6	46.313769567	31.887254789	37.978981505
6	46.503114119	31.448707971	39.368177027
6	46.216565803	34.234547861	36.892470629
6	46.083832024	30.977554579	36.815258112
7	46.690709613	30.492706862	42.200625446
7	46.518722048	32.475547784	44.251864099
7	46.715192241	34.525493809	42.258098207
7	46.637348755	32.564938675	40.218901380
1	46.434874776	29.394444235	39.021098649
1	46.490415405	29.283773253	45.368052426
1	46.693098160	35.648074651	45.437191719
1	46.879131279	35.731030132	39.087610059
1	46.868746408	26.257387330	40.900847693
1	46.659962107	27.370870805	39.551987998
1	46.597599558	33.466160556	48.605442543
1	47.234301682	38.844439762	41.105438614
1	45.396628563	30.166353617	37.077281153
1	45.636420603	31.545819616	36.000506307
1	45.321435498	35.771460259	47.019034366
1	45.779709076	35.712248113	48.806201903
1	48.926552865	36.934147560	39.366207503
1	48.675513829	38.753836880	39.182737094
1	45.425667975	26.877755382	44.098000807
1	46.757525972	26.129231004	43.230840759
1	47.088628408	27.125712950	44.650231272
1	46.442571108	31.258776424	48.556848254

1	45.160922804	30.454494619	47.666691496
1	46.828179061	29.926332998	47.468614880
1	47.530744168	38.762913487	43.453454118
1	48.252540591	37.615083329	44.572667725
1	46.515234320	37.947251773	44.639320621
1	45.932020152	33.743429087	35.961721176
1	47.168712511	34.745994783	36.709104362
1	45.462482688	34.996232829	37.120273888
26	46.608657553	32.515637516	42.230174915
6	44.710908804	32.293594462	42.014757753
1	44.401564945	32.386744819	40.973551403
6	43.863831138	31.200315044	42.598244315
8	43.672766818	30.192054565	41.941833101
8	43.411463252	31.379033949	43.847437952
6	42.580788366	30.284213254	44.355558370
6	42.240251392	30.580588117	45.799334656
1	41.689529025	30.220880294	43.724773263
1	43.138882951	29.351346939	44.244273030
1	41.682697622	31.517164610	45.888925084
1	43.139122488	30.654417847	46.418192632
1	41.624905666	29.767795098	46.196625589
6	41.998177900	36.237796005	38.511603677
6	42.153822830	36.002330122	39.878602536
6	42.403275165	34.707881072	40.377047477
6	42.517506679	33.658164424	39.445696593
6	42.428637413	33.899798731	38.073515586
6	42.154140643	35.188104261	37.605656185
1	41.784900455	37.242358350	38.166213449
1	42.102799136	36.850891929	40.556519910
1	42.686327583	32.640275190	39.786001110
1	42.559592648	33.085182385	37.368431877
1	42.053320455	35.367910911	36.540351087
14	42.630369719	34.484462586	42.224790892
1	43.868946626	33.506648685	42.403584368
6	43.304379378	36.054825330	42.984260565
1	43.426688068	35.929277837	44.062643644
1	42.618872311	36.887414721	42.808307262
1	44.268990343	36.322398059	42.546030602
6	41.187396353	33.717425047	43.143284986
1	40.383492930	34.453246308	43.263989215
1	41.484785384	33.403048342	44.147020184
1	40.772237380	32.850871907	42.619443574
1	52.987302643	31.729557313	43.409512139
1	45.270445354	26.821441345	40.498330616
1	47.001659080	30.527168726	36.437351513

PD_{css}**QM/MM Energy = -2762.488900 a.u.**

6	52.125598492	31.819564547	43.921640450
1	52.312672550	32.454166858	44.797793041
1	51.861706762	30.823080352	44.283685564
6	50.977505994	32.333056496	43.116094467
7	51.005151198	33.395554060	42.236331200
1	51.819480746	33.985289835	41.993401424
6	49.754048718	33.611135082	41.787440082
1	49.520442252	34.382759931	41.072881126
7	48.905502850	32.741916994	42.338560486
6	49.666539555	31.930303136	43.156882142
1	49.235399451	31.118418514	43.720120880
6	46.531754451	30.358443746	39.981032534
6	46.608561618	30.448435158	44.804768750
6	47.003324999	35.263708439	44.702649892
6	46.891042493	35.173192638	39.881620195
6	46.550639644	29.956087339	41.358051803
6	46.367277928	28.557781348	41.781755608

6	46.407214723	28.577522306	43.140595225	1	46.948018102	30.430389045	47.712883664
6	46.589087731	29.991479983	43.525244605	1	47.700204196	39.111849928	43.277757365
6	46.193680617	27.443592279	44.086710541	1	48.430770738	38.046447789	44.466752110
6	46.132279032	27.364565716	40.903341954	1	46.687001414	38.349984653	44.501149954
6	46.661309255	31.823096811	45.196238590	1	45.973523847	33.829021174	36.051612653
6	46.570465174	32.249008612	46.600531697	1	47.210763650	34.846388205	36.774456207
6	46.651282129	33.613807935	46.586002310	1	45.502802925	35.119225872	37.169982592
6	46.808077904	34.001175937	45.166145497	26	46.936474979	32.800171784	42.334221995
6	46.335335678	31.334475209	47.762379697	6	42.130041859	31.405879402	41.887499737
6	46.608730457	34.489435100	47.753501532	1	41.149047597	31.030396308	41.580337242
6	46.087469552	35.723763878	47.842565523	6	42.575944167	30.655632092	43.105345565
6	47.099262336	35.651823538	43.322885749	8	43.673696414	30.144909365	43.250012993
6	47.332394755	37.032416982	42.909870447	8	41.619684910	30.628391825	44.058980960
6	47.397066332	37.010663267	41.541623587	6	41.958863062	29.958875415	45.298745849
6	47.115697063	35.613217745	41.145958282	6	42.777521645	30.857337531	46.207535843
6	47.544536416	38.189150139	43.837146772	1	40.995846788	29.702221708	45.742898750
6	47.698451323	38.129163808	40.654593996	1	42.504873868	29.041291548	45.069553769
6	48.509193880	38.073506527	39.583568212	1	42.273901096	31.814356681	46.370983513
6	46.619011297	33.808005497	39.507468475	1	43.758398318	31.046737762	45.764464167
6	46.371200883	33.398021116	38.117354090	1	42.913722519	30.367814539	47.175403746
6	46.321921458	32.036048652	38.128263079	6	41.937363697	36.256971071	39.232466166
6	46.509367496	31.637290079	39.534254512	6	41.871405541	35.568135214	40.446094731
6	46.254228406	34.347447674	36.968930619	6	42.077239378	34.174243843	40.520284529
6	46.070672424	31.097254769	36.989200414	6	42.408645197	33.513587897	39.324836632
7	46.686495330	30.800188176	42.387250625	6	42.504888484	34.196976102	38.106990524
7	46.785761187	32.858106400	44.358163123	6	42.247800836	35.566878106	38.056070761
7	46.986734567	34.809064461	42.290558490	1	41.762175446	37.328195482	39.199434160
7	46.665555802	32.776360348	40.353521903	1	41.671610782	36.130522220	41.359323877
1	46.444462187	29.568625953	39.247597042	1	42.601886346	32.445303483	39.332641864
1	46.516321912	29.718875091	45.600134734	1	42.758466602	33.653662644	37.201176120
1	47.093640675	36.061406110	45.429556342	1	42.295543229	36.099598774	37.110592289
1	46.942717376	35.898969734	39.078122244	14	41.893984974	33.283806843	42.186466325
1	46.643283006	26.498562031	41.338422280	1	42.854064330	31.203479682	41.095715400
1	46.523946599	27.489614798	39.892054454	6	43.194352395	33.969000230	43.383534695
1	47.035158783	34.052876496	48.655429822	1	43.112808631	33.489247368	44.364392609
1	47.289284870	39.094234157	40.951482769	1	43.044565975	35.045636473	43.527864842
1	45.401399398	30.285610605	37.290498271	1	44.215612261	33.825421303	43.014452630
1	45.593847775	31.640621906	36.173045300	6	40.187864700	33.543619309	42.937281966
1	45.589045550	36.211825796	47.010701216	1	40.052554163	34.560334363	43.322278645
1	46.130670482	36.272021422	48.778800057	1	40.063714378	32.862035938	43.784308847
1	49.031328288	37.172301474	39.272478829	1	39.385640056	33.320984672	42.225936042
1	48.726923055	38.978982162	39.026104772	1	53.087218150	31.731569202	43.416059823
1	45.129100544	27.349417980	44.338350447	1	45.080036923	27.085948952	40.846539131
1	46.497839100	26.494482445	43.639806590	1	46.981258175	30.645461839	36.595774365
1	46.744366746	27.568141659	45.022910461				
1	46.551766506	31.829355094	48.712223103				
1	45.290525699	31.006918074	47.800705746				