

TABLE S1 *Pseudomonas putida* NCIB 9816 NDO substrates

Spiro, Bridged-linked, and Bridged Ring Structures

There are no known substrates in these three ring categories.

Direct-linked Isolated Ring Structures

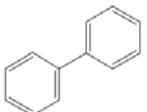
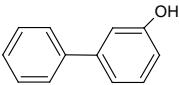
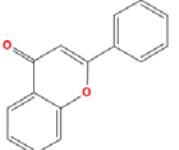
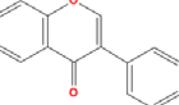
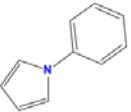
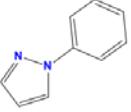
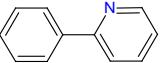
Substrate Name	Structure	Reference
biphenyl		(1)
3-hydroxy biphenyl		(2)
flavone		(3)
isoflavone		(3)
1-phenylpyrrole		(4, 5)
1-phenylpyrazole		(4, 5)
2-phenyl pyridine		(5)

TABLE S1 NDO substrates (con't.)

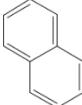
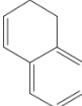
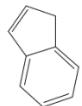
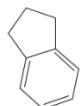
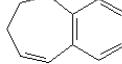
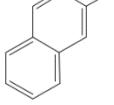
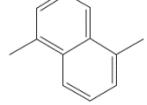
Fused Ring Structures		
Substrate Name	Structure	Reference
naphthalene		(6)
1,2-dihydronaphthalene		(7)
indene		(8)
indan		(8)
6,7-dihydro-5H-benzocycloheptene		(9)
norcarane		(10)
bicyclo[3.1.0]hexane		(10)
2-methyl naphthalene		(11)
1,5-dimethyl naphthalene		(12)

TABLE S1 NDO substrates (con't.)

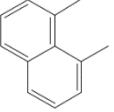
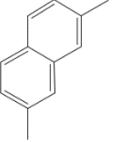
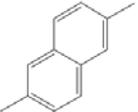
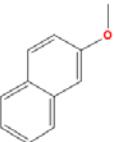
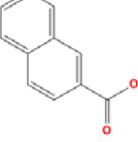
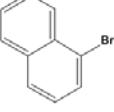
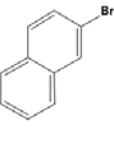
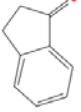
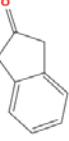
Fused Ring Structures (con't.)		
Substrate Name	Structure	Reference
1,8-dimethyl naphthalene		(12)
2,7-dimethyl naphthalene		(12)
2,6-dimethyl naphthalene		(12)
2-methoxy naphthalene		(13)
2-naphthoic acid		(1)
1-bromonaphthalene		(14)
2-bromonaphthalene		(14)
1-indanone		(15)
2-indanone		(15)

TABLE S1 NDO substrates (con't.)

Fused Ring Structures (con't.)		
Substrate Name	Structure	Reference
(1 <i>R</i>)-indanol		(16)
(1 <i>S</i>)-indanol		(16)
(1 <i>R</i>)-indenol		(16)
(1 <i>S</i>)-indenol		(16)
anthracene		(17)
9,10-dihydroanthracene		(18)
phenanthrene		(17)
9,10-dihydrophenanthrene		(18)
fluorene		(19)

TABLE S1 NDO substrates (con't.)

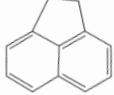
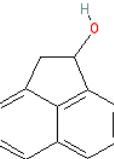
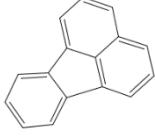
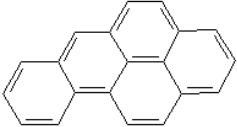
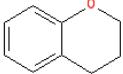
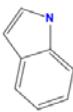
Fused Ring Structures (con't.)		
Substrate Name	Structure	Reference
acenaphthylene		(12)
acenaphthene		(12)
acenaphthen-1-ol		(12)
fluoranthene		(20)
benzo[a]pyrene		(20)
Heterocyclic Fused Ring Structures		
Substrate Name	Structure	Reference
chromane		(21)
indole		(22)

TABLE S1 NDO substrates (con't.)

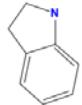
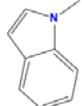
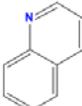
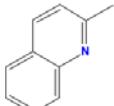
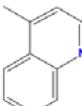
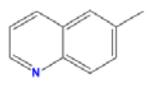
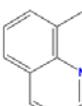
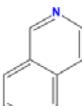
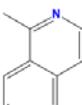
Heterocyclic Fused Ring Structures (con't.)		
Substrate Name	Structure	Reference
indoline		(1)
N-methylindole		(1)
quinoline		(23)
2-methylquinoline		(23)
4-methylquinoline		(23)
6-methylquinoline		(23)
8-methylquinoline		(23)
isoquinoline		(23)
1-methylisoquinoline		(23)

TABLE S1 NDO substrates (con't.).

Heterocyclic Fused Ring Structures (con't.)		
Substrate Name	Structure	Reference
3-methylisoquinoline		(23)
phthalazine		(23)
cinnoline		(23)
quinazoline		(23)
quinoxaline		(23)
1,5-naphthyridine		(23)
benzothiophene		(24)
2-methylbenzothiophene		(24)
3-methylbenzothiophene		(1)

TABLE S1 NDO substrates (con't.)

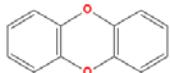
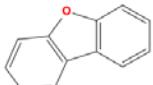
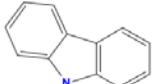
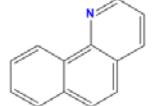
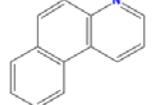
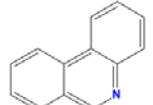
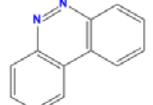
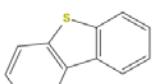
Heterocyclic Fused Ring Structures (con't.)		
Substrate Name	Structure	Reference
dibenzo-1,4-dioxin		(25)
dibenzofuran		(19)
carbazole		(26)
Benzo[<i>h</i>]quinoline		(5)
Benzo[<i>f</i>]quinoline		(5)
Phenanthridine		(5)
Benzo[<i>c</i>]cinnoline		(5)
dibenzothiophene		(19)

TABLE S1 NDO substrates (con't.)

Single Ring Structures		
Substrate Name	Structure	Reference
benzene		(27)
toluene		(28)
ethylbenzene		(28)
o-xylene		(28)
m-xylene		(28)
p-xylene		(28)
styrene		(29)
1,2,4-trimethylbenzene		(12)
dimethylfulvene		(30)

TABLE S1 NDO substrates (con't.)

Single Ring Structures (con't.)		
Substrate Name	Structure	Reference
1,3 cyclohexadiene		(30)
1,3 cycloheptadiene		(30)
cycloheptatriene		(30)
1,3 cyclooctadiene		(30)
phenol		(31)
o-cresol		(31)
m-cresol		(31)
p-cresol		(31)
(S)-1-phenethyl alcohol		(28)

TABLE S1 NDO substrates (con't.)

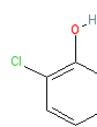
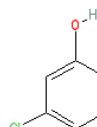
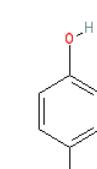
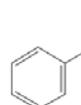
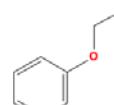
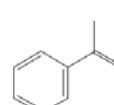
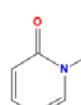
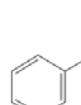
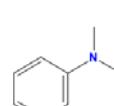
Single Ring Structures (con't.)		
Substrate Name	Structure	Reference
2-chlorophenol		(31)
3-chlorophenol		(31)
4-chlorophenol		(31)
anisole		(12, 32)
phenetole		(12, 32)
acetophenone		(28)
1-methylpyridin-2-one		(33)
N-methylaniline		(1)
N,N-dimethylaniline		(1)

TABLE S1 NDO substrates (con't.).

Single Ring Structures (con't.)		
Substrate Name	Structure	Reference
o-nitrotoluene		(28)
p-nitrotoluene		(28)
m-nitrotoluene		(28)
methyl phenyl sulfide		(34, 35)
ethyl phenyl sulfide		(34, 35)
n-propyl phenyl sulfide		(35)
i-propyl phenyl sulfide		(35)
n-butyl phenyl sulfide		(35)
ethenyl phenyl sulfide		(35)

TABLE S1 NDO substrates (con't.)

Single Ring Structures (con't.)		
Substrate Name	Structure	Reference
methyl p-tolyl sulfide		(34, 35)
p-methoxyphenyl methyl sulfide		(34, 35)
p-fluorophenyl methyl sulfide		(35)
p-chlorophenyl methyl sulfide		(35)
p-bromophenyl methyl sulfide		(35)
p-chlorophenyl ethyl sulfide		(35)
m-chlorophenyl methyl sulfide		(35)
o-chlorophenyl methyl sulfide		(35)
methyl p-nitrophenyl sulfide		(34, 35)

TABLE S1 NDO substrates (con't.)

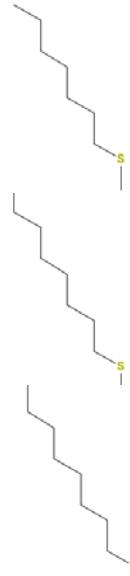
Single Ring Structures (con't.)		
Substrate Name	Structure	Reference
methyl p-cyanophenyl sulfide		(35)
benzyl methyl sulfide		(35)
benzyl ethyl sulfide		(35)
[2-(methylsulfanyl)ethyl] benzene		(35)
methyl thiocyclohexane		(35)
o-bromostyrene		(36)

TABLE S1 NDO substrates (con't.)

Non-Ring Structures		
Substrate Name	Structure	Reference
methylthiohexane		(35)

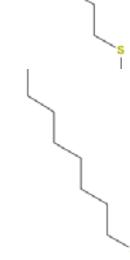
methylthioheptane

(35)



methylthiooctane

(35)



methylthiononane

(35)



References

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TABLE S2 Composition of three water mixtures used to assay Pseudomonas NCIB 9816-4 activity

Mixture #1	μg/mL	Mixture #2	μg /mL	Mixture #3	μg /mL
1,1-diphenylethylene	0.2	aniline	1.6	tetralin	2.3
quinoline	0.2	cyclooctane	1.3	cyclopropylbenzene	2.3
benzothiophene	0.2	isododecane	1.2	1-phenyl napthalene	2.6
1,2,3-trimethylbenzene	0.2	1,2 dimethylnaphthalene	0.8	<i>cis</i> -stilbene	2.4
1,3,5-trimethylbenzene	0.2	indan	0.8	isochroman	2.6
1,2,4-trimethylbenzene	0.2	p-cymene	0.7	2,3 benzofuran	2.6
bicyclohexane	0.2	1,2,3,4-tetrahydroquinoline	0.8	spiro[2.4]hepta-4,6-diene	2.2
1,4-diisopropylbenzene	0.2	<i>cis</i> -decalin	0.7	norbornadiene	2.2
acenaphthene	0.5	<i>trans</i> -decalin	0.7	fluorene	3.2
acenaphthylene	0.2	diphenyl sulfide	0.9	fluoranthene	1.2
admantane	0.3	azulene	0.8	<i>m</i> -terphenyl	0.9
bibenzyl	0.3	1-methylphenanthrene	0.6	benzophenone	2.2
biphenylene	0.1	naphthalene	1.5	diphenylmethane	2.2
pyrene	0.6	hexa-methyl benzene	1.1	xanthene	3.0
triphenylene	0.3	diphenyl ether	1.6		
triphenylmethane	0.2	norbornane	0.9		
<i>trans</i> -stilbene	0.6	norbornylene	1.3		
biphenyl	0.6				
fluorene	0.4				
phenanthrene	0.5				

TABLE S3 Estimated relative product yields^a

Substrate	product 1	product 2	product 3	unreacted
spiroheptadiene	1	<1		5
spiro [cyclopropane-1,1'-indene]	2	3		not detected
diphenyl methane	50			50
cyclohexylbenzene	80	10		10
phenylnaphthalene	5	10	85	30
diphenyl ether	6			10
cyclopropylbenzene	1	1	1	45
1,1-diphenylethylene	15	15	40	10
tetralin	2			not detected
<i>trans</i> -decalin	4	3		55

^a Reported as percent of starting material GC/FID peak area. Products are listed in the same order as in the figures with corresponding mass spectra.

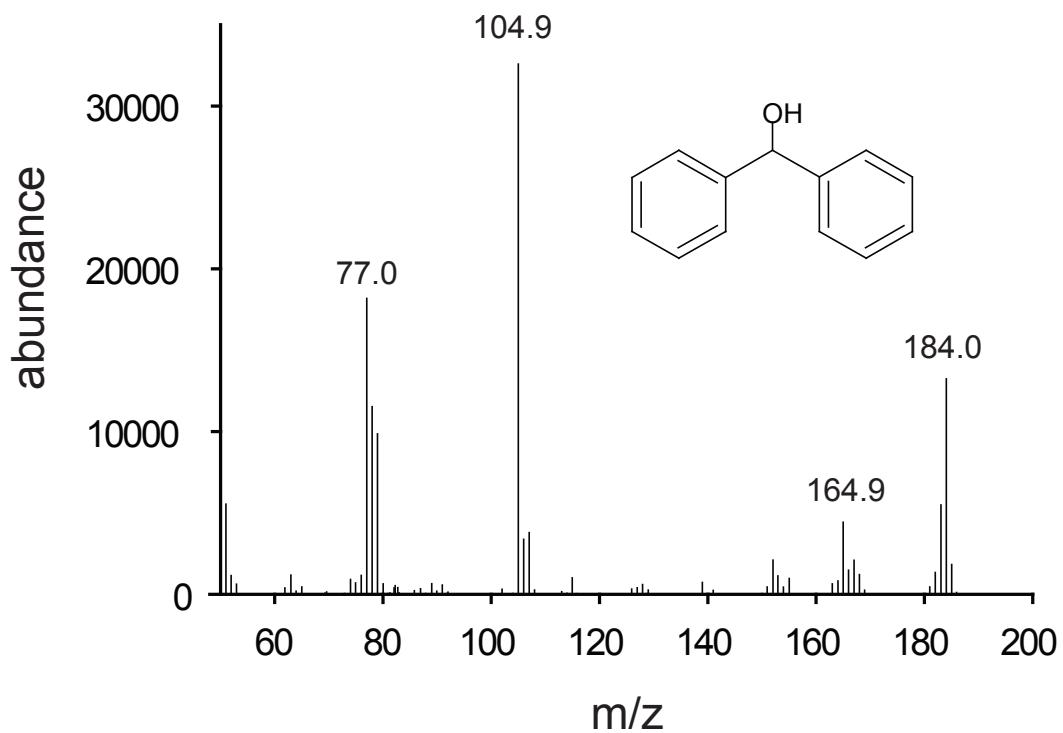


Figure S1 Mass spectrum of product of NDO reaction with diphenylmethane putatively identified as diphenylmethanol.

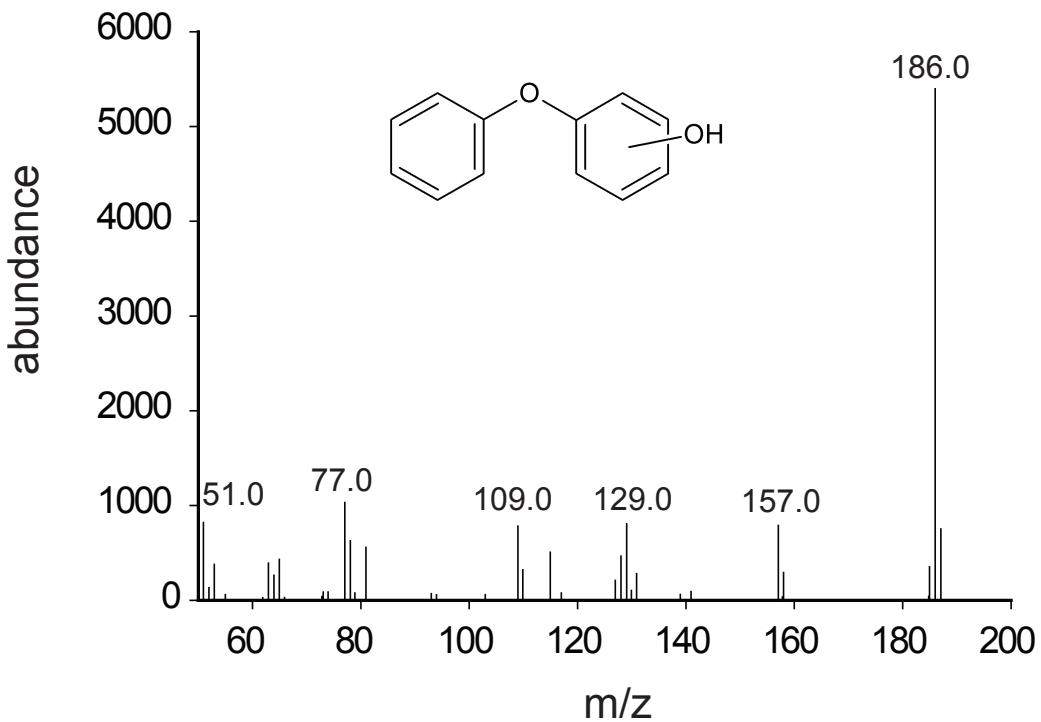


Figure S2 Mass spectrum of product of NDO reaction with diphenyl ether putatively identified as a phenoxy phenol. The exact position of the hydroxyl group was not determined.

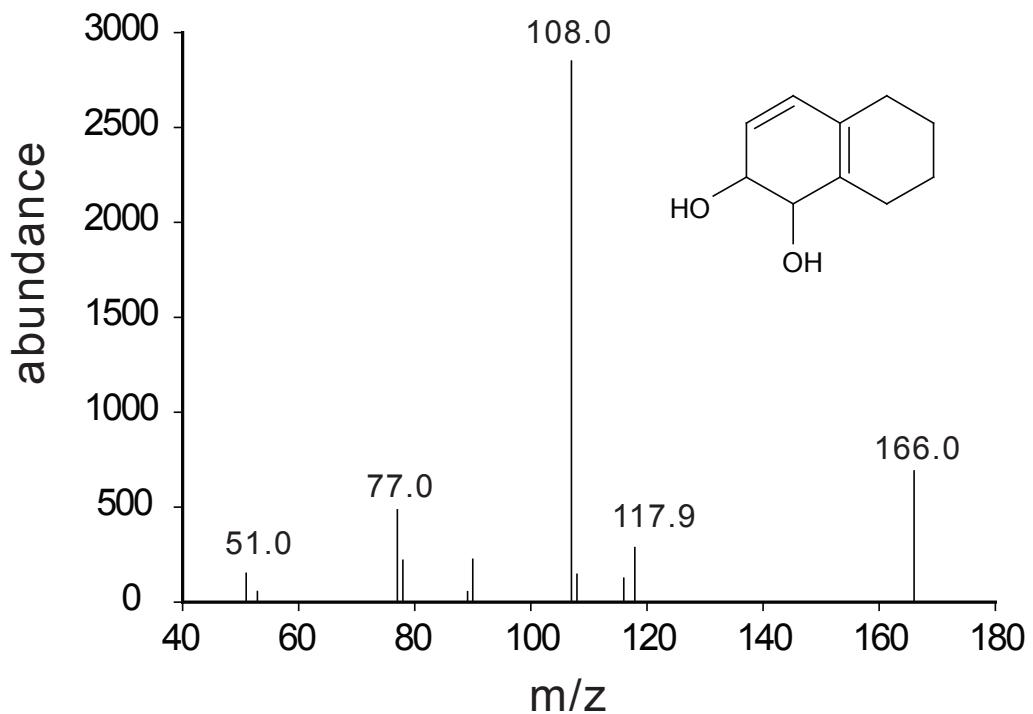
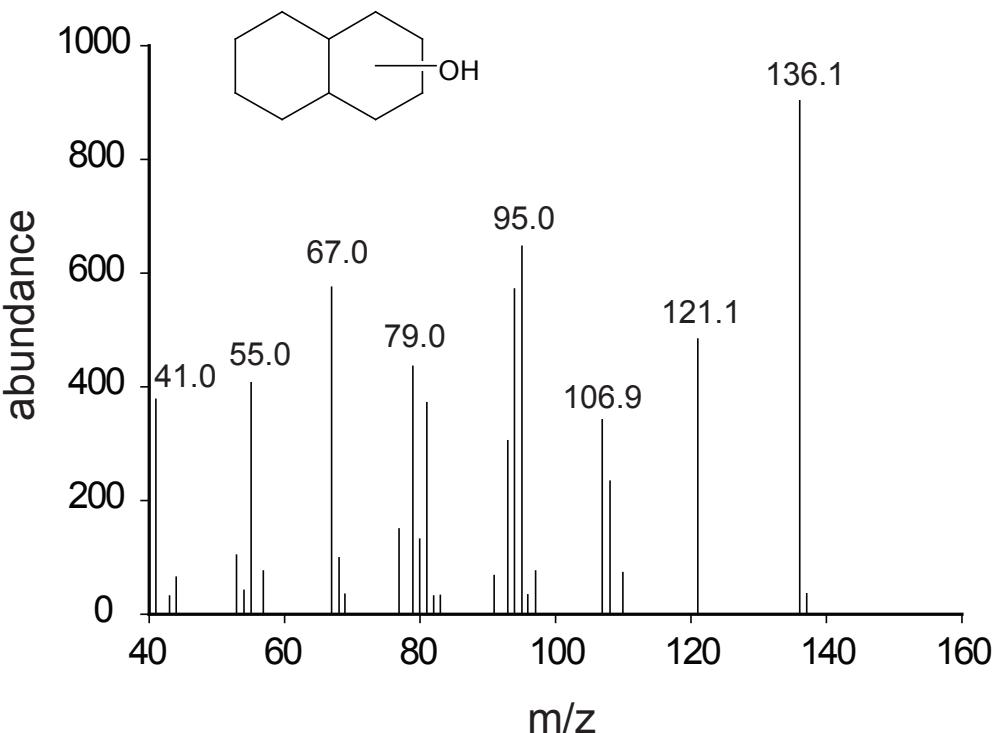


Figure S3 Mass spectrum of product of NDO reaction with tetralin putatively identified as 1,2,5,6,7,8-hexahydro-1,2-naphthalenediol. The exact position of the diol was not determined and could be 2,3-naphthalenediol.

A



B

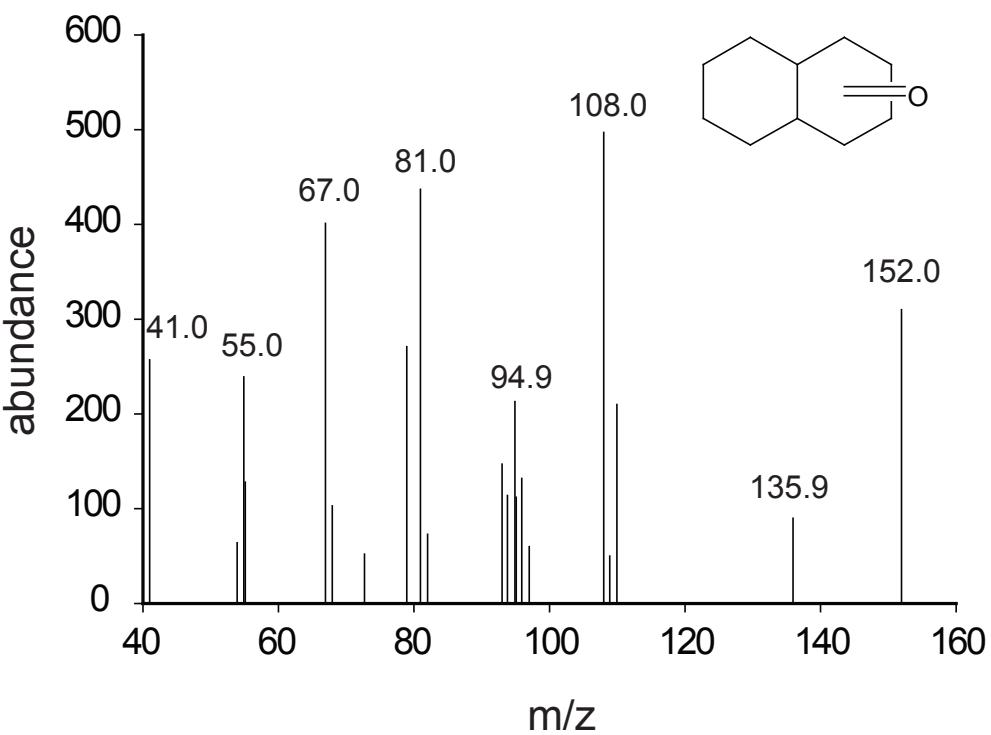


Figure S4 Mass spectra of products of NDO reaction with trans-decalin putatively identified as (A) decahydro-naphthalenol and (B) octahydro-naphthalenone. The positions of the hydroxy and ketones were not determined.