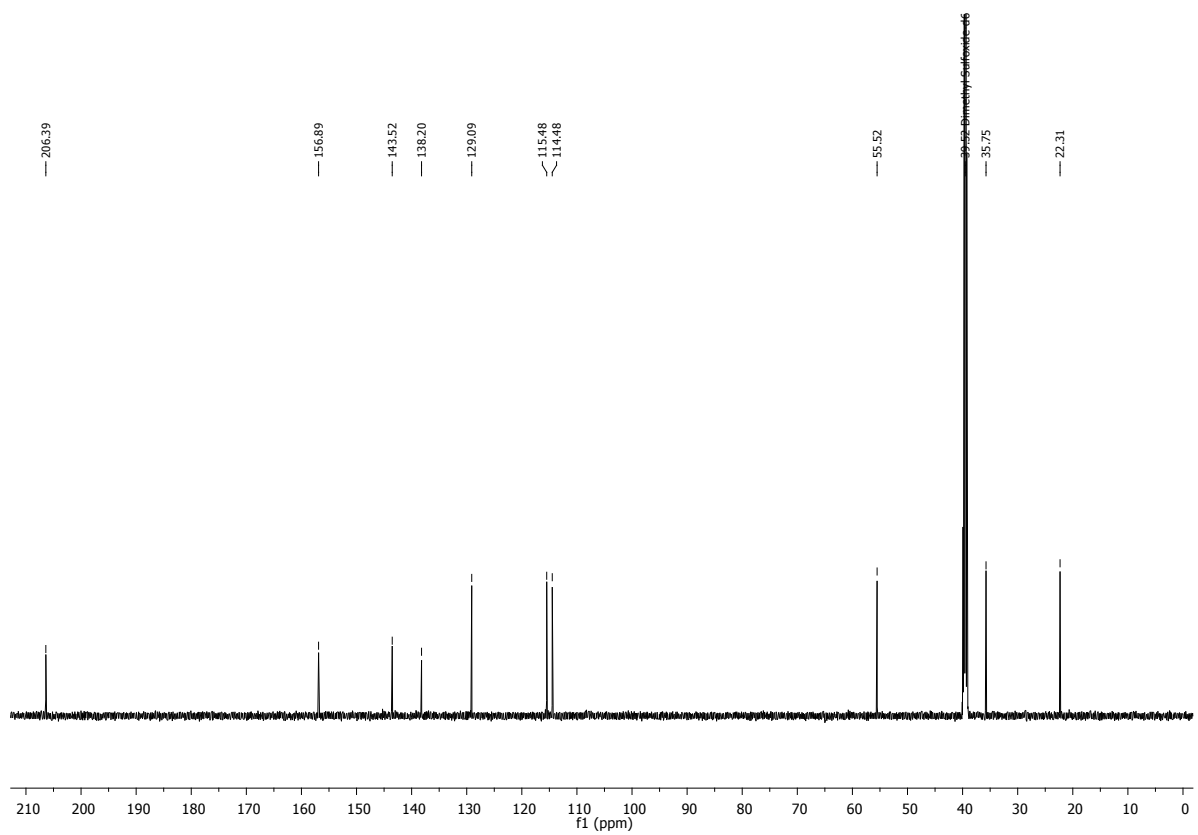
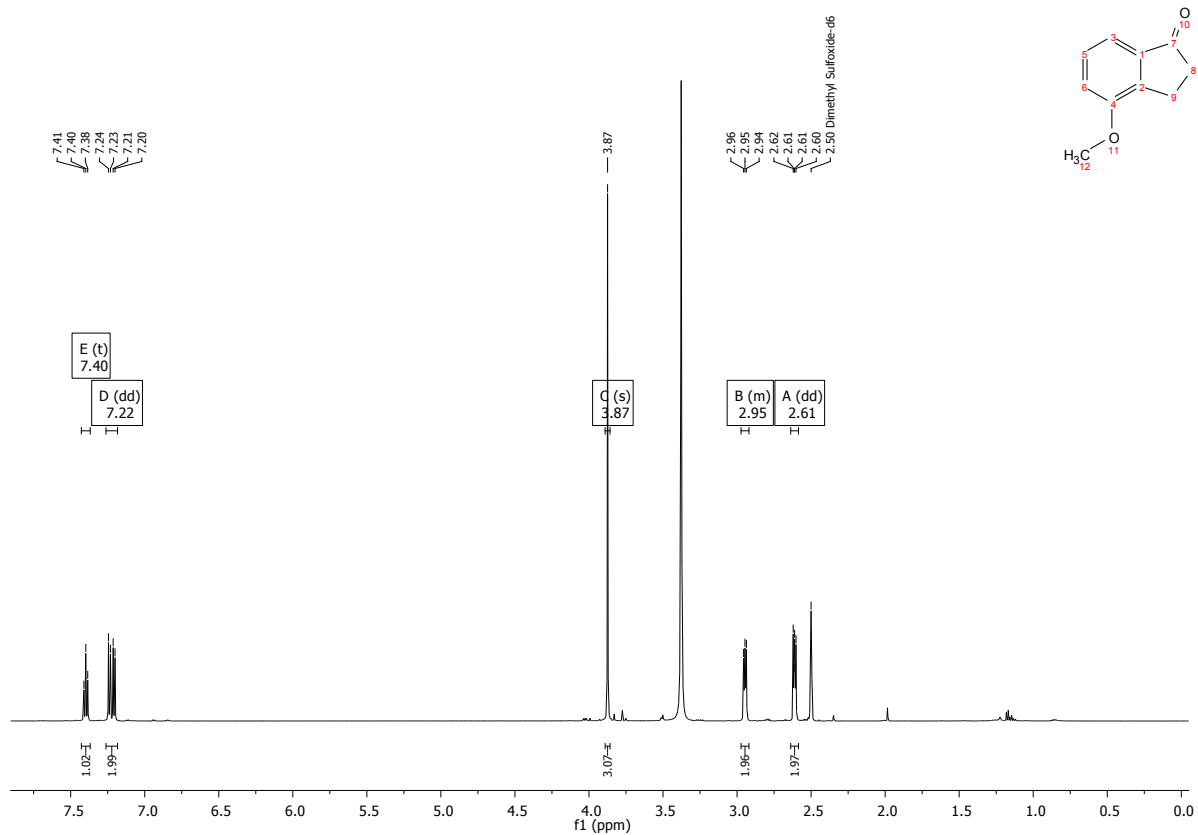


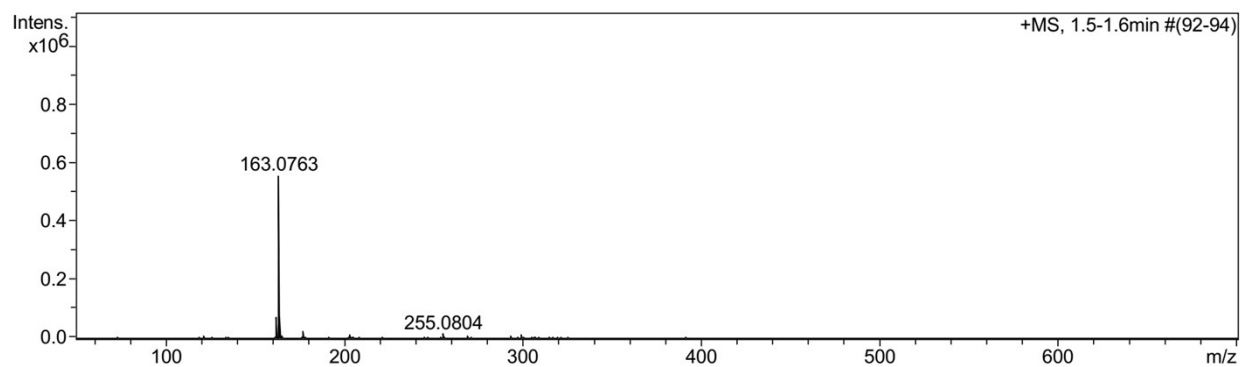
Electronic supplementary information (ESI)

4-methoxy-2,3-dihydro-1H-inden-1-one (2a):

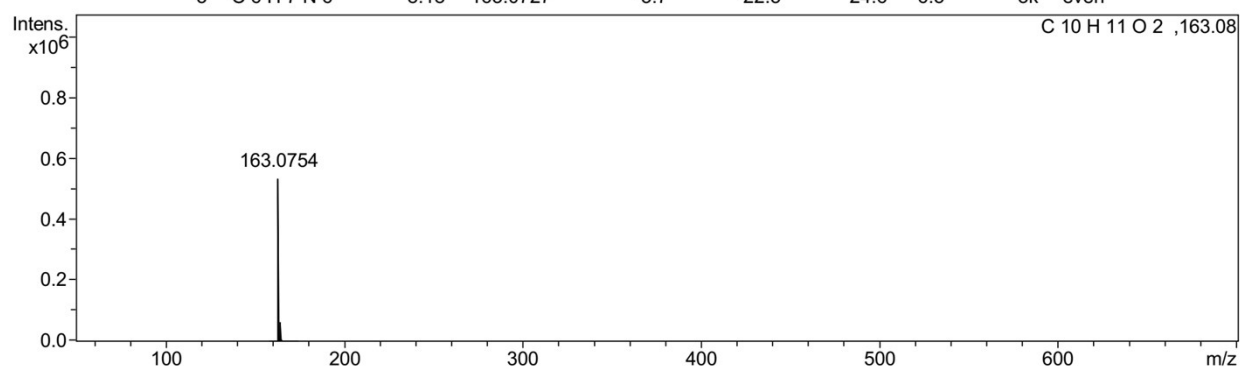
Nuclear magnetic resonance (NMR) spectra



Mass spectra (MS)

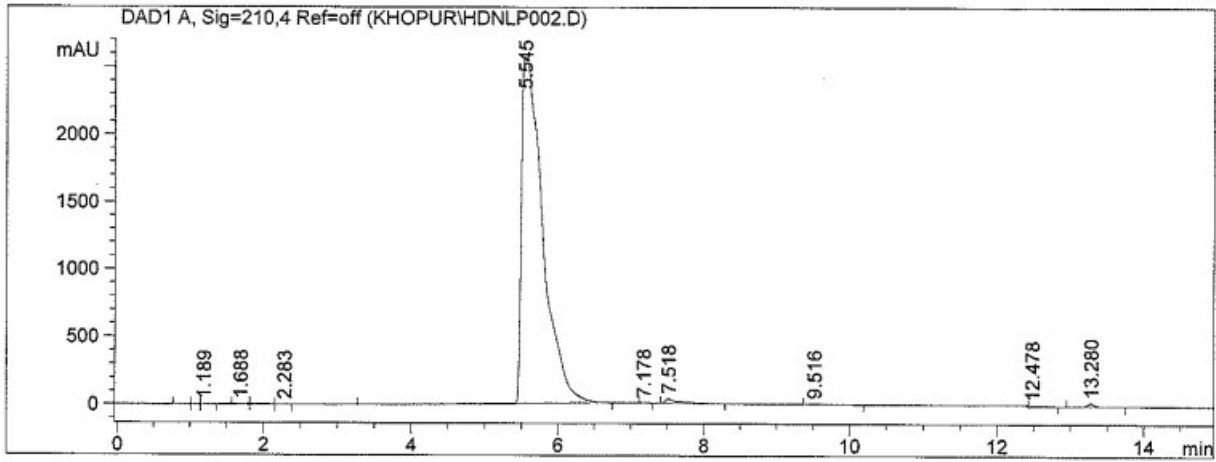


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	N-Rule	e ⁻ Conf
163.0763	1	C 10 H 11 O 2	100.00	163.0754	-1.0	-6.0	11.6	5.5	ok	even
	2	C 8 H 9 N 3 O	34.06	163.0740	-2.3	-14.2	18.8	6.0	ok	odd
	3	C 6 H 7 N 6	8.18	163.0727	-3.7	-22.5	24.6	6.5	ok	even



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	N-Rule	e ⁻ Conf
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High-performance liquid chromatography (HPLC) chromatogram



Area Percent Report

Sorted By : Signal
 Calib. Data Modified : 2013/05/28 11:12:51 AM
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

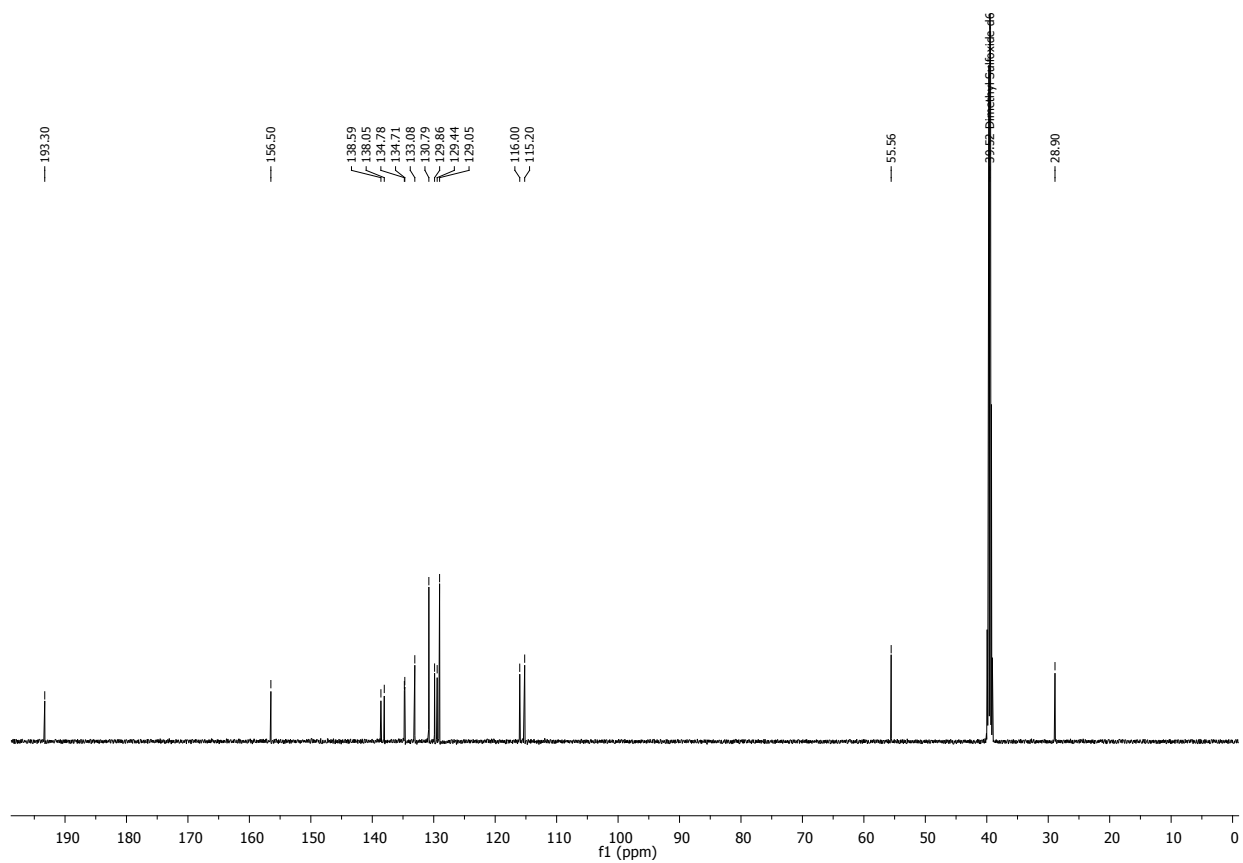
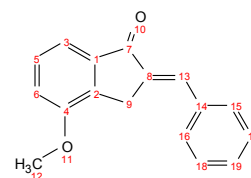
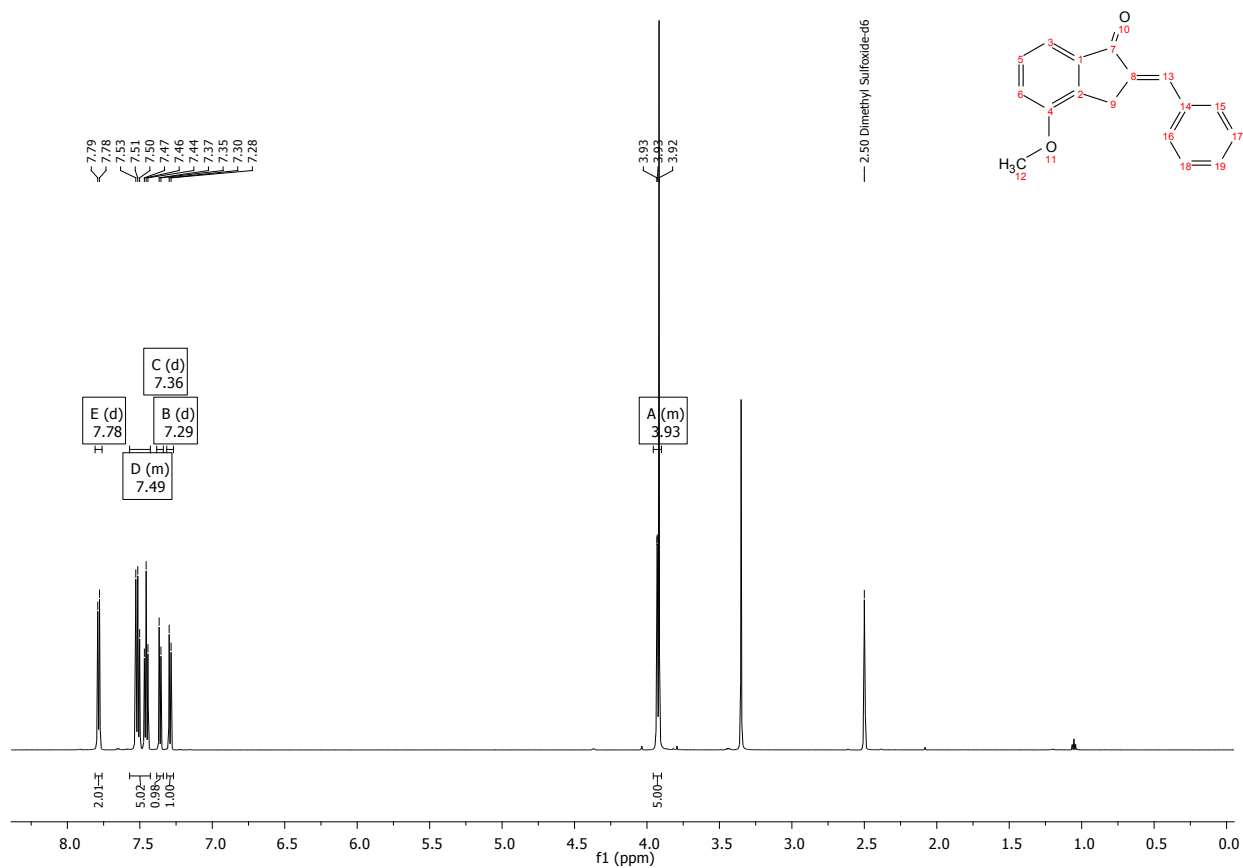
Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	0.964	VV	0.1659	15.82110	0.0304	?
2	1.051	VV	0.1018	10.15845	0.0195	?
3	1.189	VB	0.1454	16.22145	0.0312	?
4	1.688	BB	0.0777	9.63380	0.0185	?
5	1.919	BB	0.2673	32.87612	0.0632	?
6	2.283	BB	0.1193	13.34806	0.0257	?
7	2.887		0.0000	0.00000	0.0000	sulf
8	5.220		0.0000	0.00000	0.0000	pir
9	5.545	BB	0.2735	5.12667e4	98.6314	?
10	7.178	BB	0.0787	5.51010	0.0106	?
11	7.518	BB	0.1667	383.94351	0.7387	?
12	9.516	BBA	0.2102	40.98358	0.0788	?
13	12.478	PB	0.1071	36.28995	0.0698	?
14	13.280	BB	0.0937	146.60283	0.2820	?

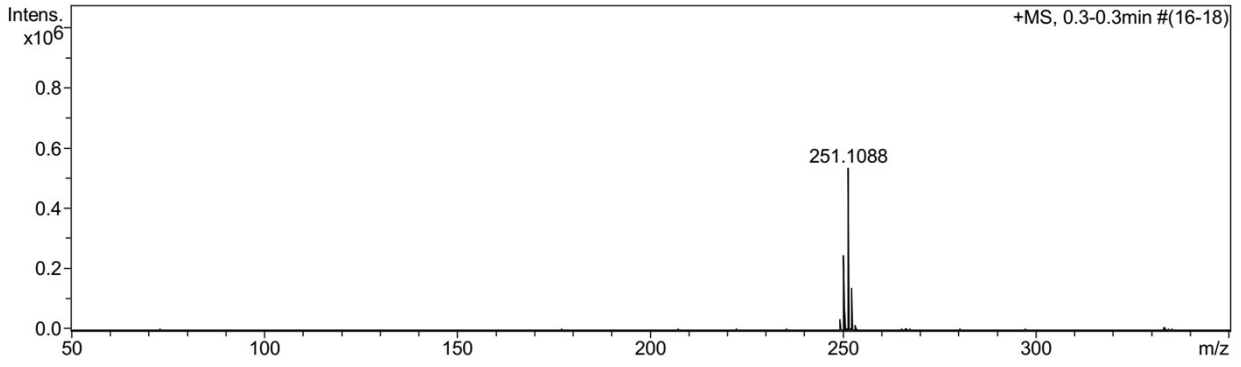
Totals : 5.19781e4

(E)-2-benzylidene-4-methoxy-2,3-dihydro-1H-inden-1-one (2b):

NMR spectra

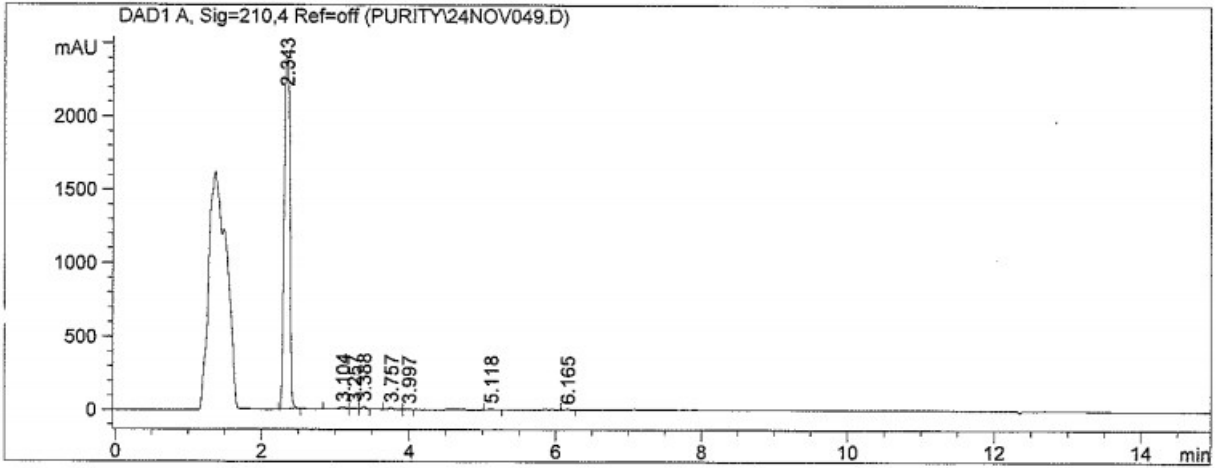


MS



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	N-Rule	e ⁻ Conf
251.1088	1	C ₁₇ H ₁₅ O ₂	100.00	251.1067	-2.2	-8.6	44.1	10.5	ok	even
	2	C ₁₀ H ₁₉ O ₇	4.75	251.1125	3.7	14.8	87.7	1.5	ok	even

HPLC chromatogram



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

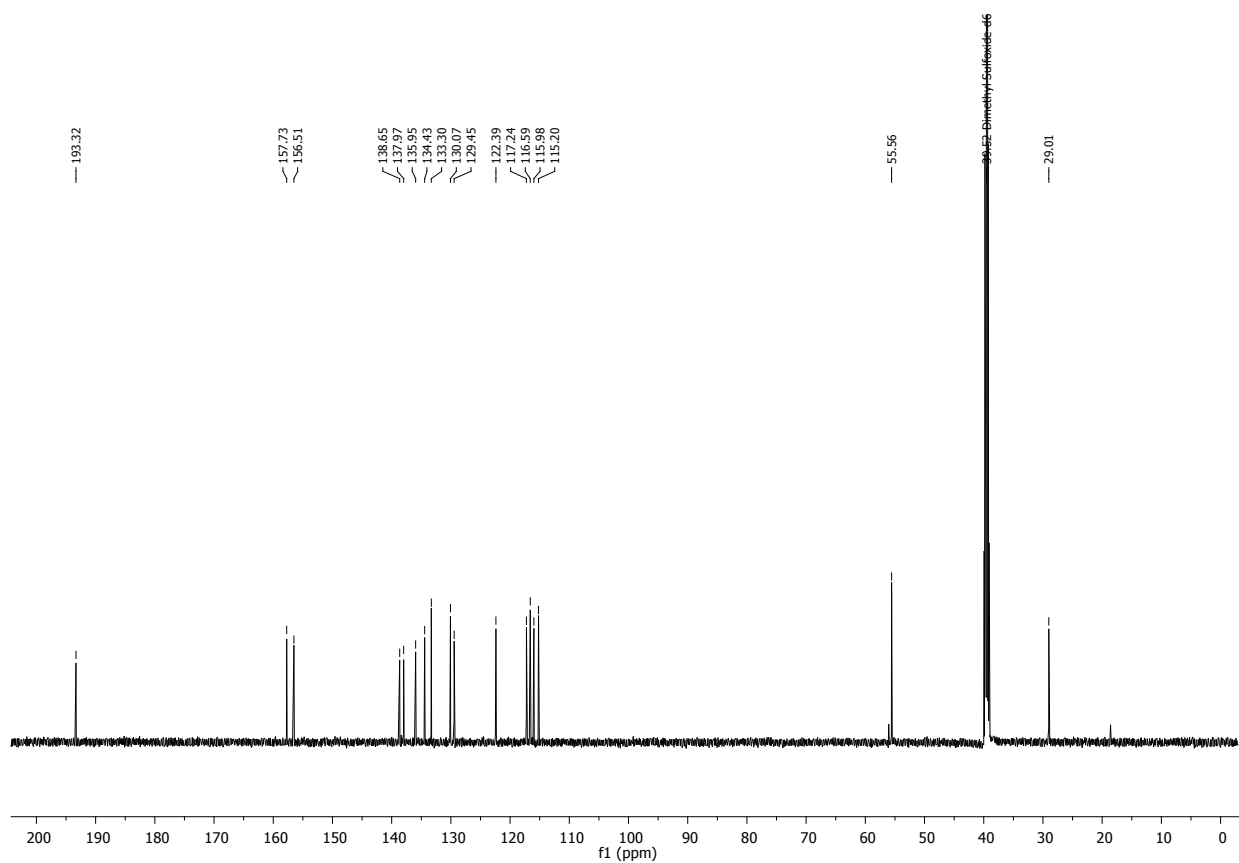
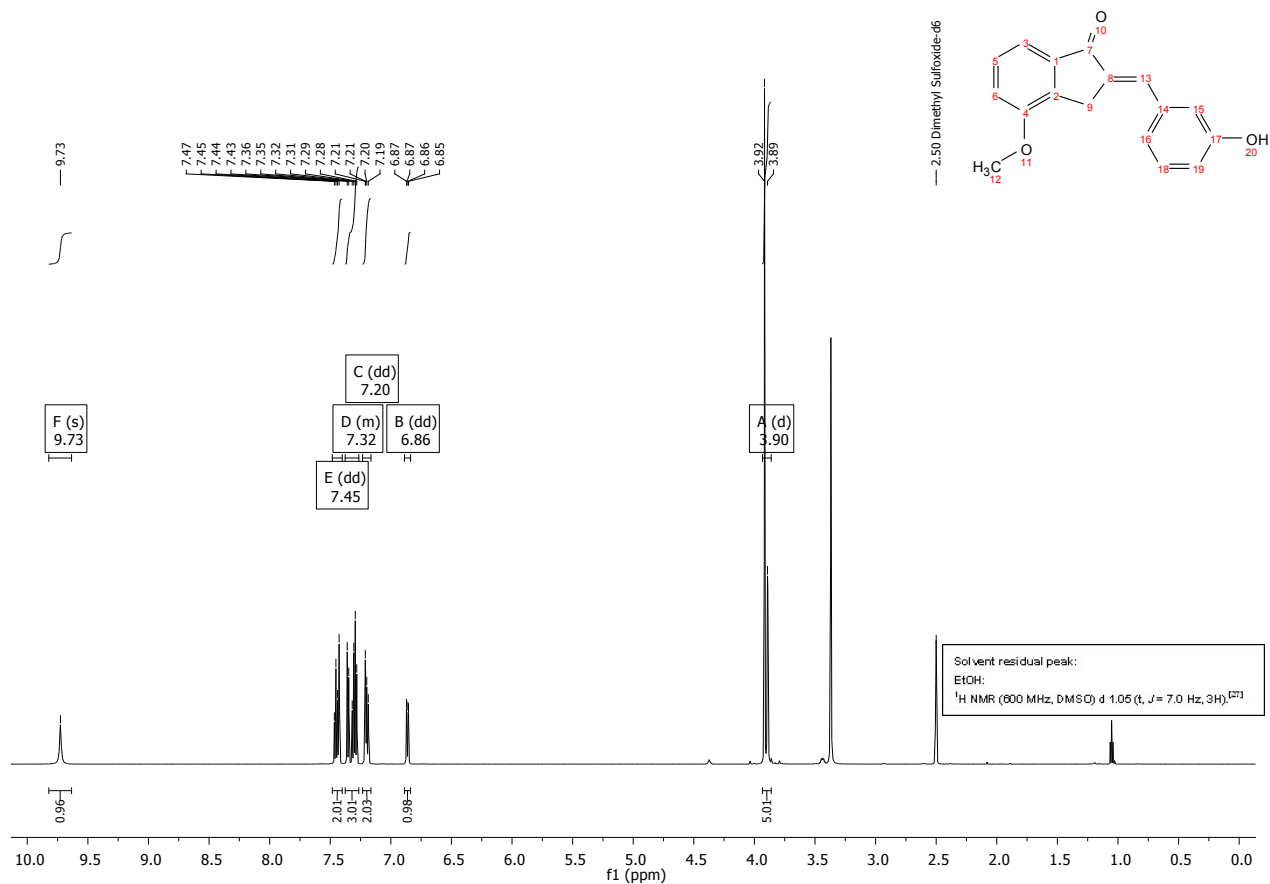
Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.343	PBA	0.0881	1.28312e4	2411.35864	98.0813
2	3.104	PB	0.0809	64.26879	12.30296	0.4913
3	3.257	BB	0.0587	21.91106	5.98245	0.1675
4	3.388	BB	0.0534	56.22673	16.63841	0.4298
5	3.757	BB	0.0697	56.11786	12.20233	0.4290
6	3.997	BB	0.0561	13.94288	4.05715	0.1066
7	5.118	PBA	0.0647	25.13927	6.02553	0.1922
8	6.165	BBA	0.0607	13.40537	3.50096	0.1025

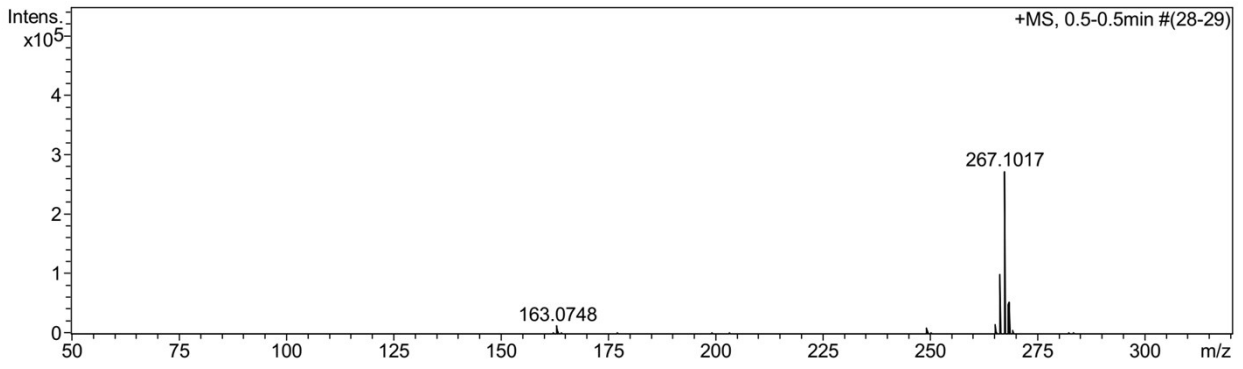
Totals : 1.30822e4 2472.06844

(E)-2-(3-hydroxybenzylidene)-4-methoxy-2,3-dihydro-1H-inden-1-one (2c)

NMR spectra

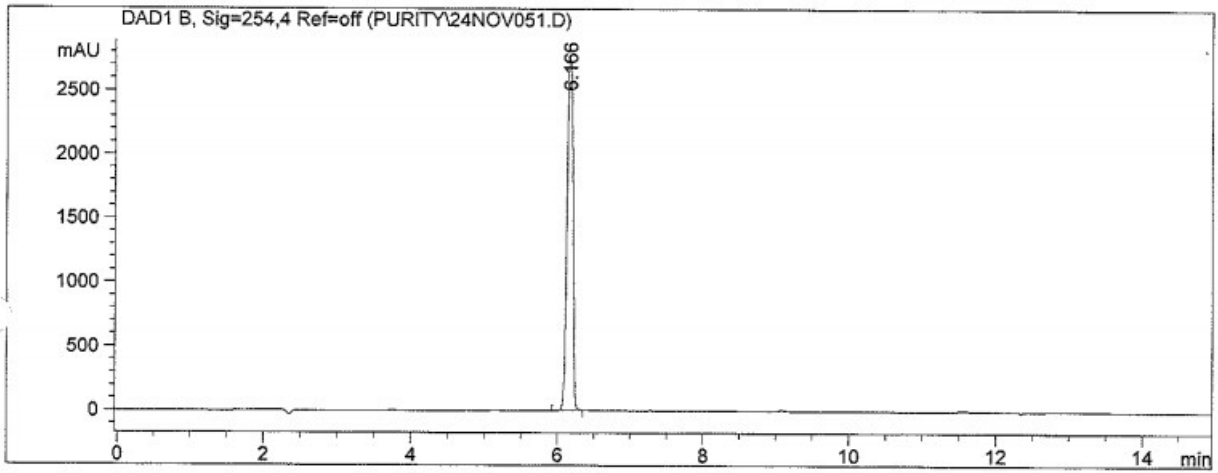


MS



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	N-Rule	e ⁻ Conf
267.1017	1	C ₁₇ H ₁₅ O ₃	100.00	267.1016	-0.1	-0.5	5.1	10.5	ok	even

HPLC chromatogram



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Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

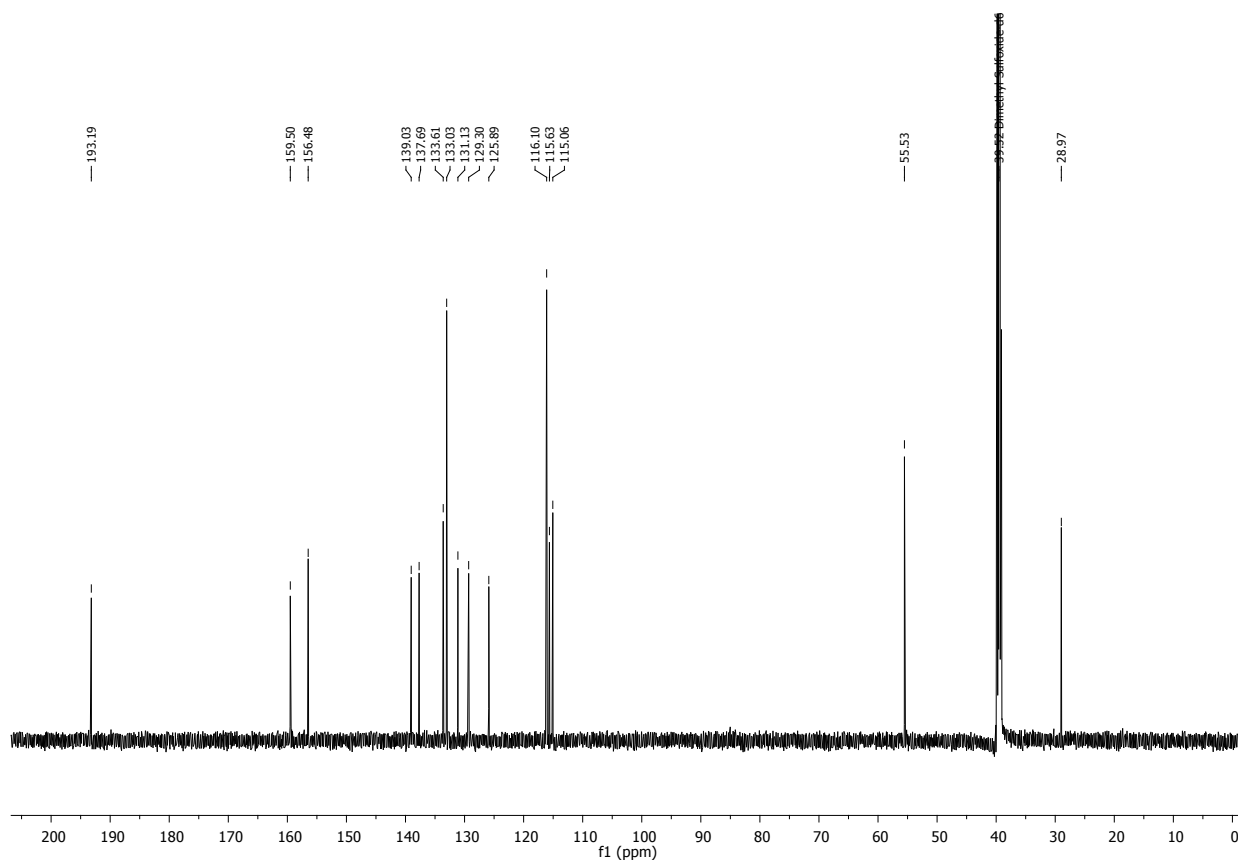
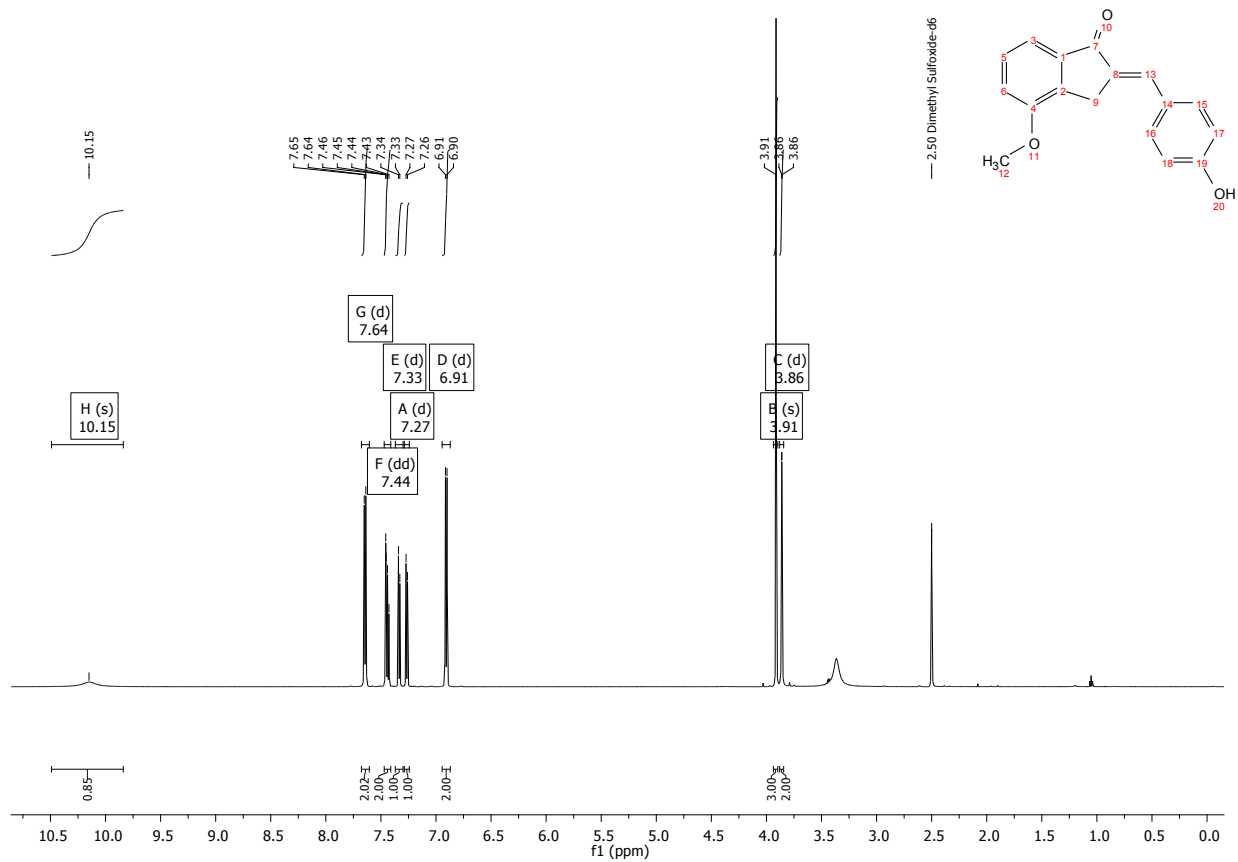
Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.166	PB	0.0941	1.55369e4	2742.97998	100.0000

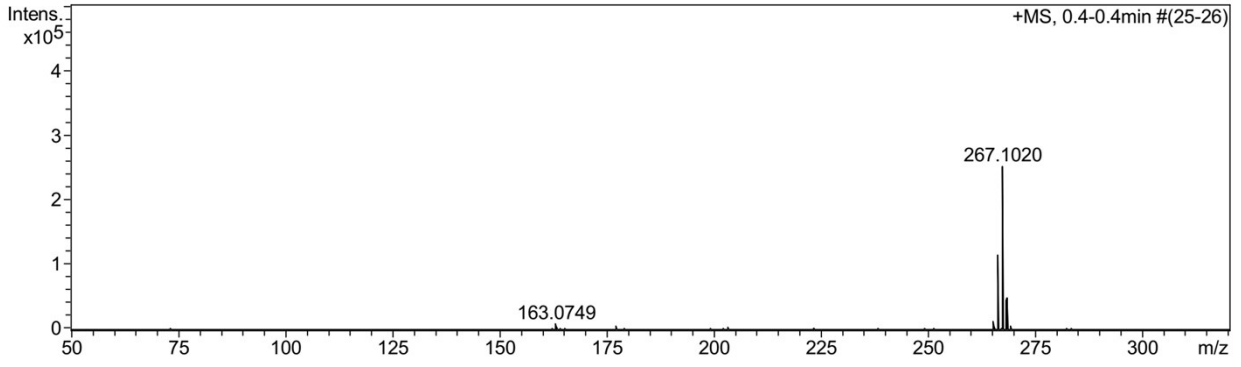
Totals : 1.55369e4 2742.97998

(E)-2-(4-hydroxybenzylidene)-4-methoxy-2,3-dihydro-1H-inden-1-one (2d)

NMR spectra

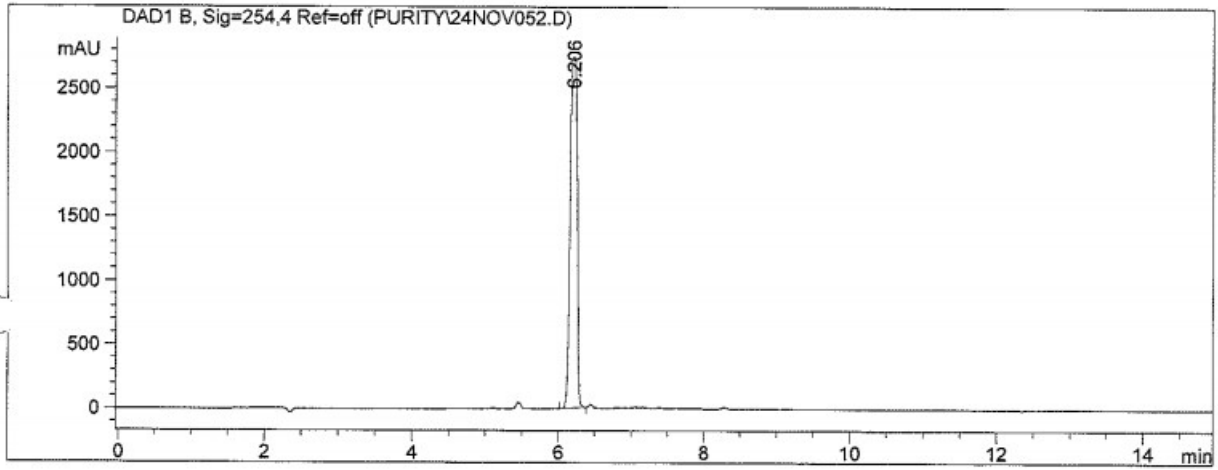


MS



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	N-Rule	e ⁻ Conf
267.1020	1	C ₁₇ H ₁₅ O ₃	100.00	267.1016	-0.4	-1.5	4.9	10.5	ok	even

HPLC chromatogram



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

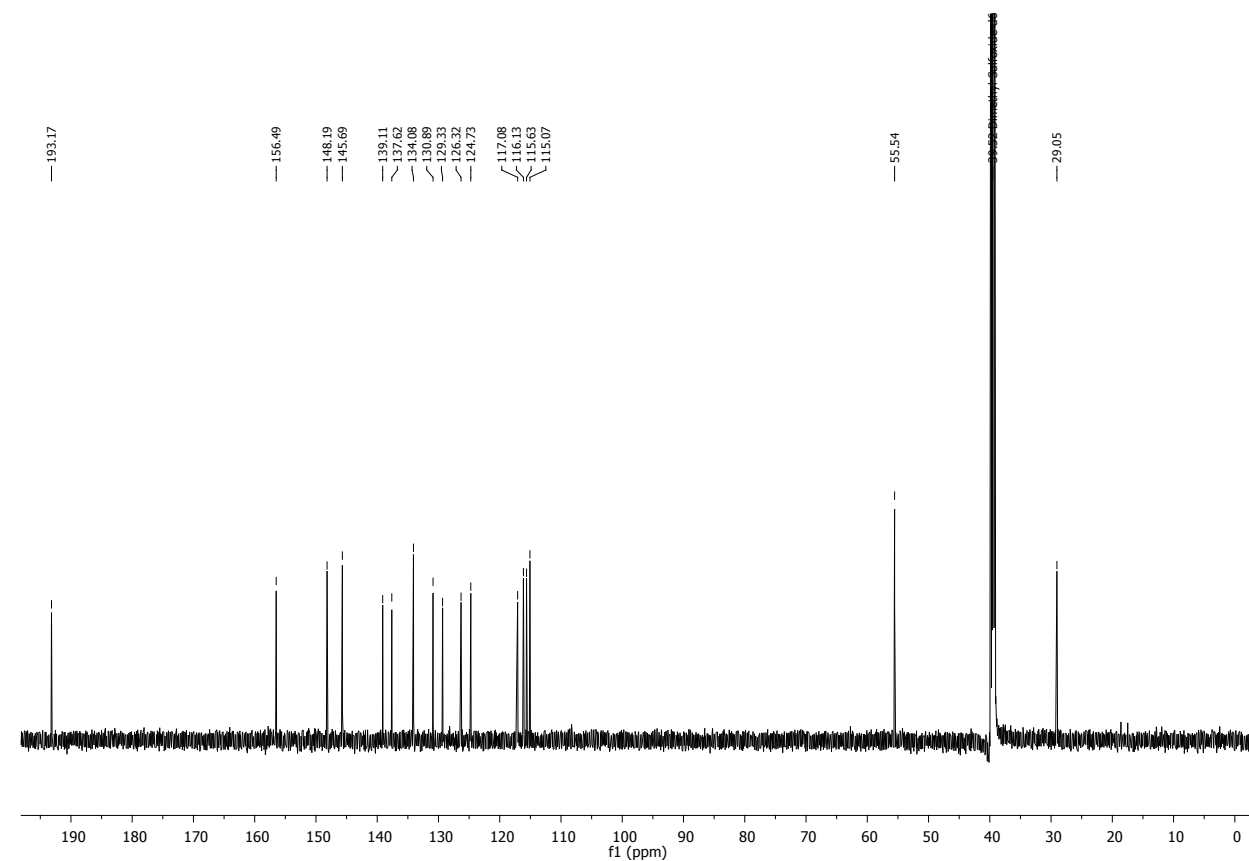
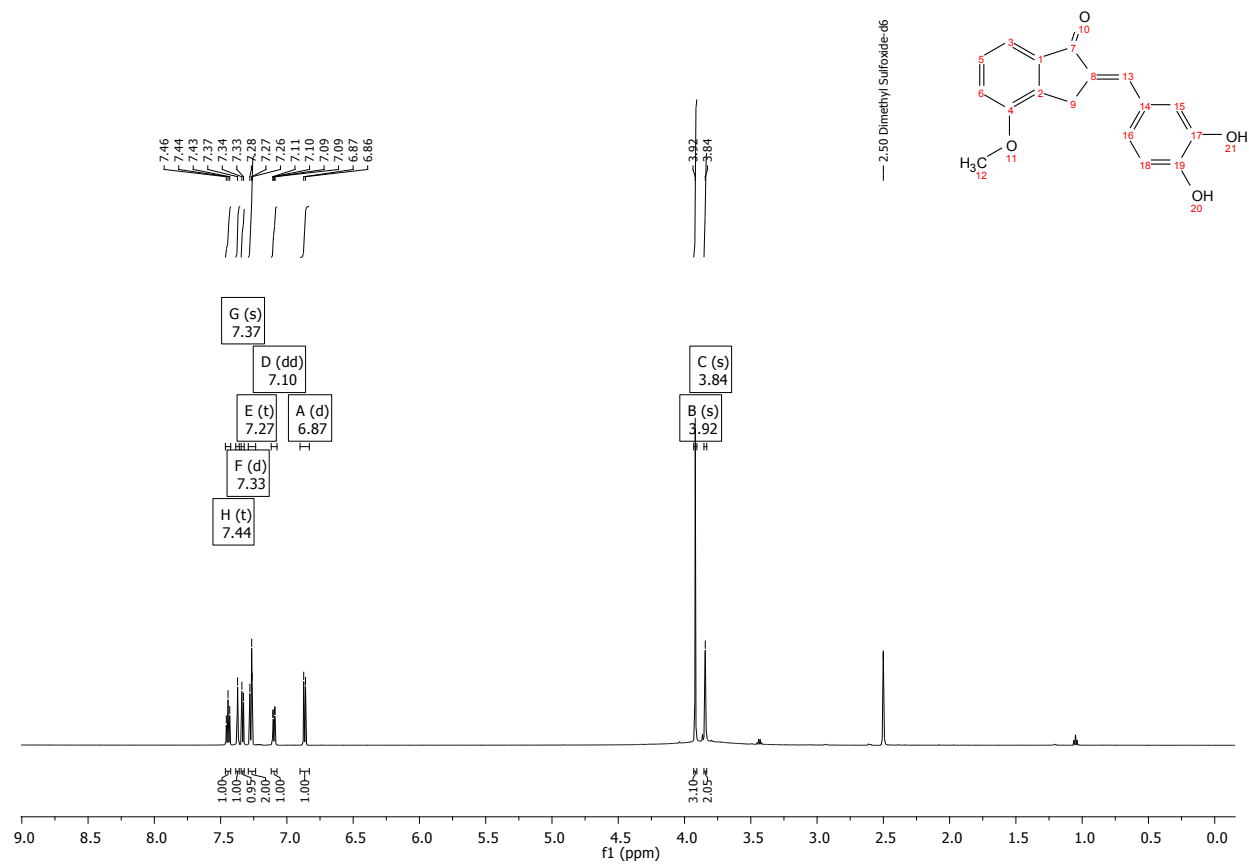
Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.206	BB	0.1092	1.81342e4	2740.04321	100.0000

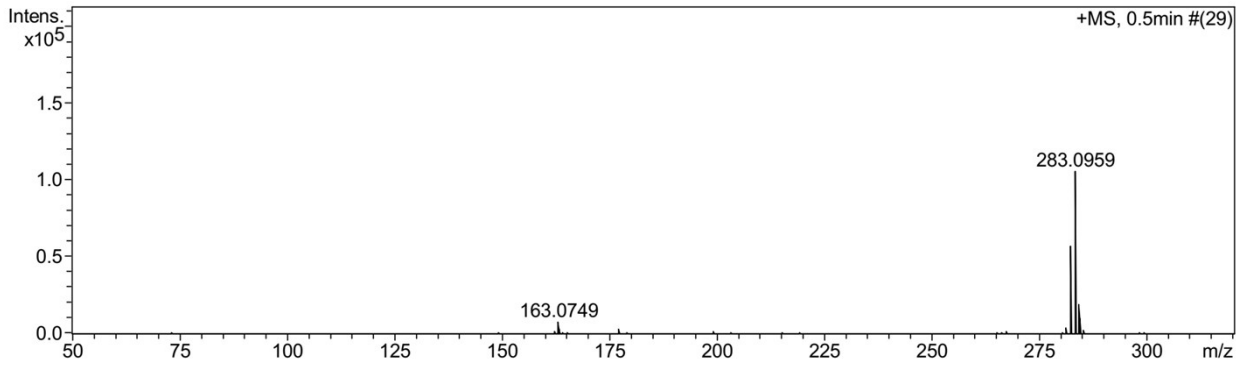
Totals : 1.81342e4 2740.04321

(E)-2-(3,4-dihydroxybenzylidene)-4-methoxy-2,3-dihydro-1H-inden-1-one (2e)

NMR spectra

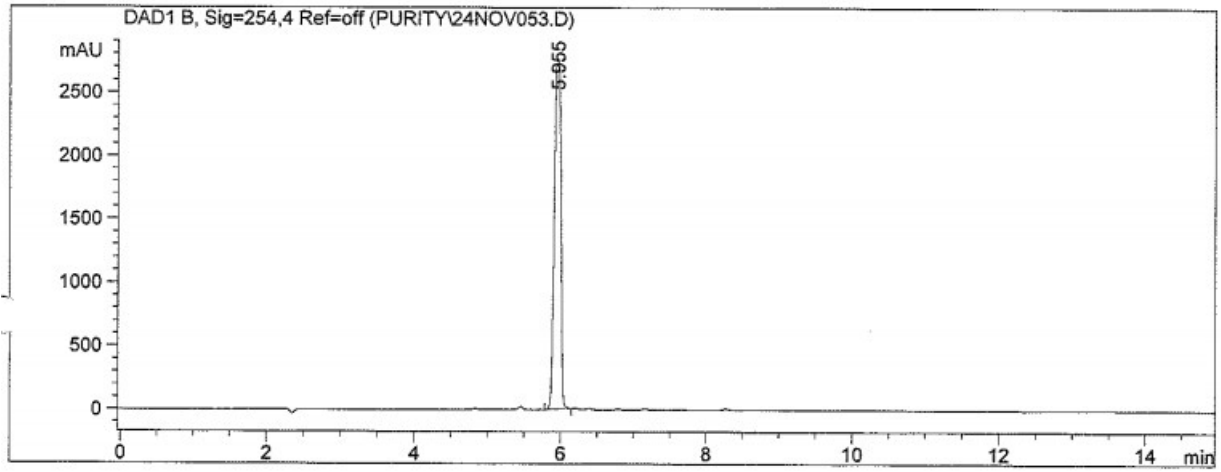


MS



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	N-Rule	e ⁻ Conf
283.0959	1	C ₁₇ H ₁₅ O ₄	100.00	283.0965	0.6	2.0	0.7	10.5	ok	even

HPLC chromatogram



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

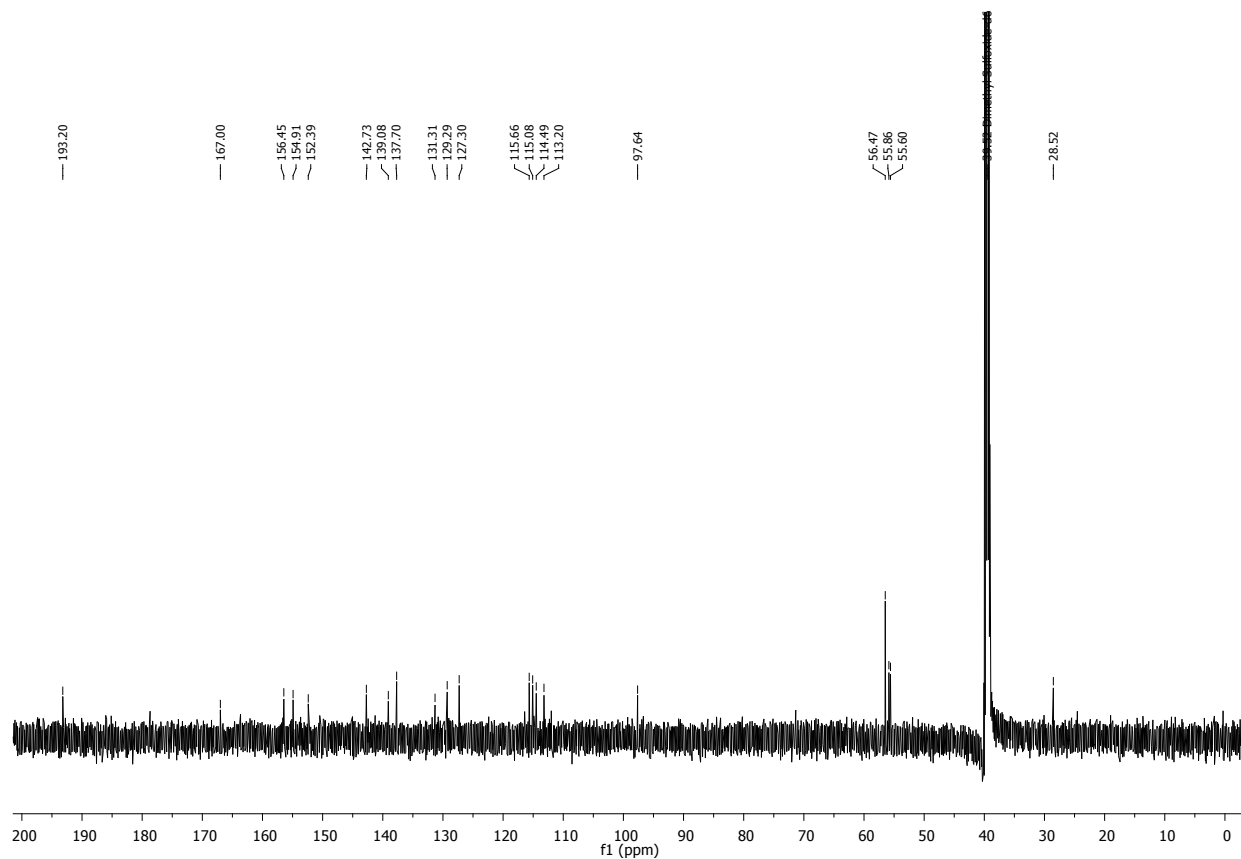
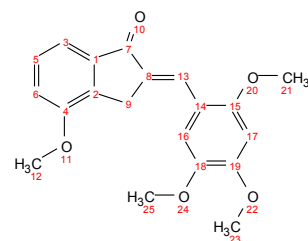
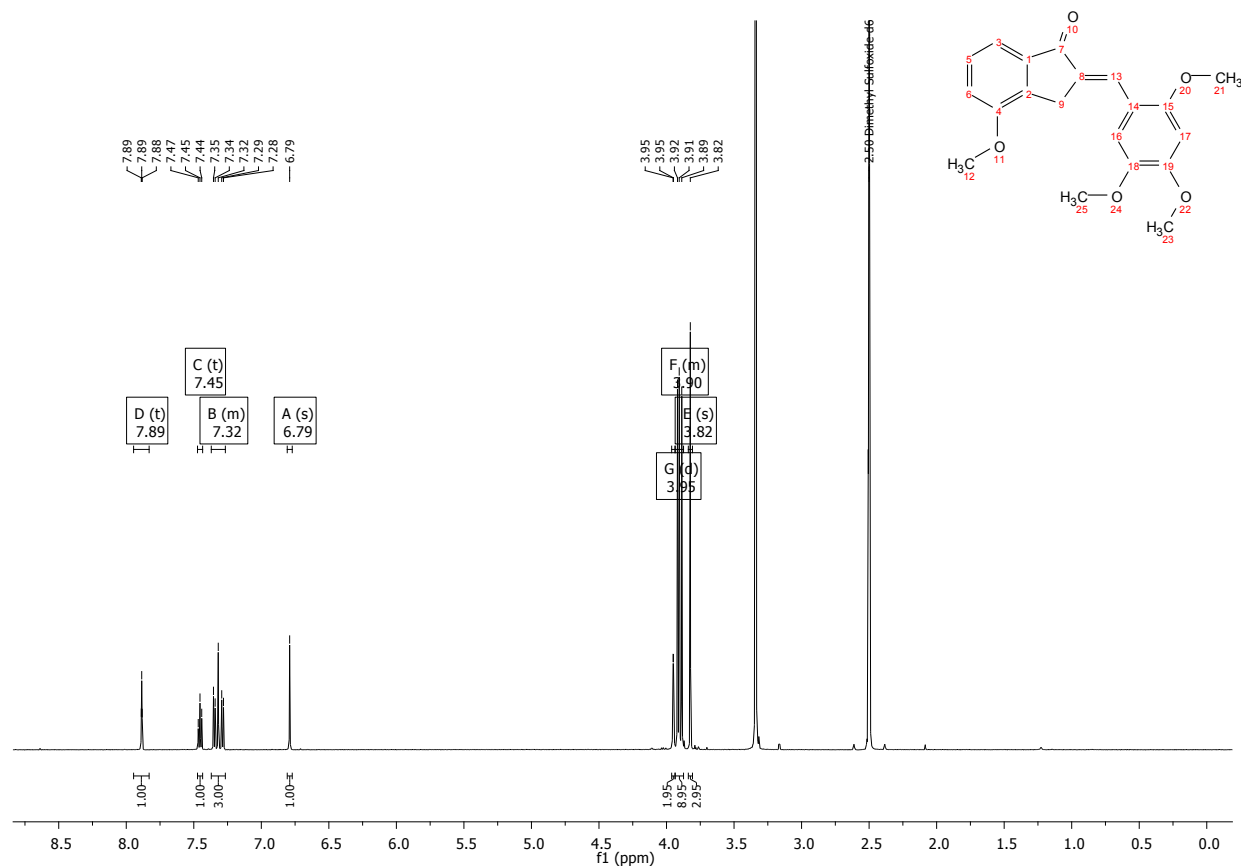
Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.955	PB	0.1022	1.70845e4	2762.24927	100.0000

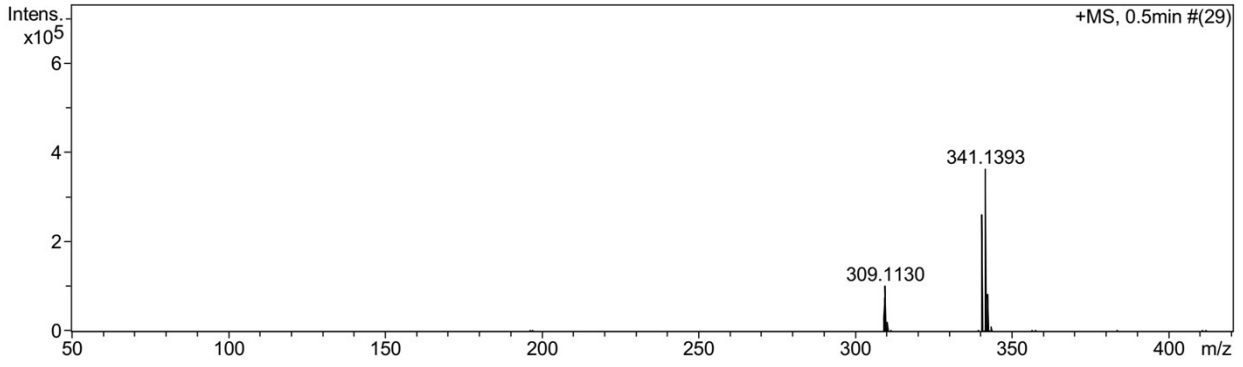
Totals : 1.70845e4 2762.24927

(E)-2-(2,4,5-trimethoxybenzylidene)-4-methoxy-2,3-dihydro-1H-inden-1-one (2f)

NMR spectra

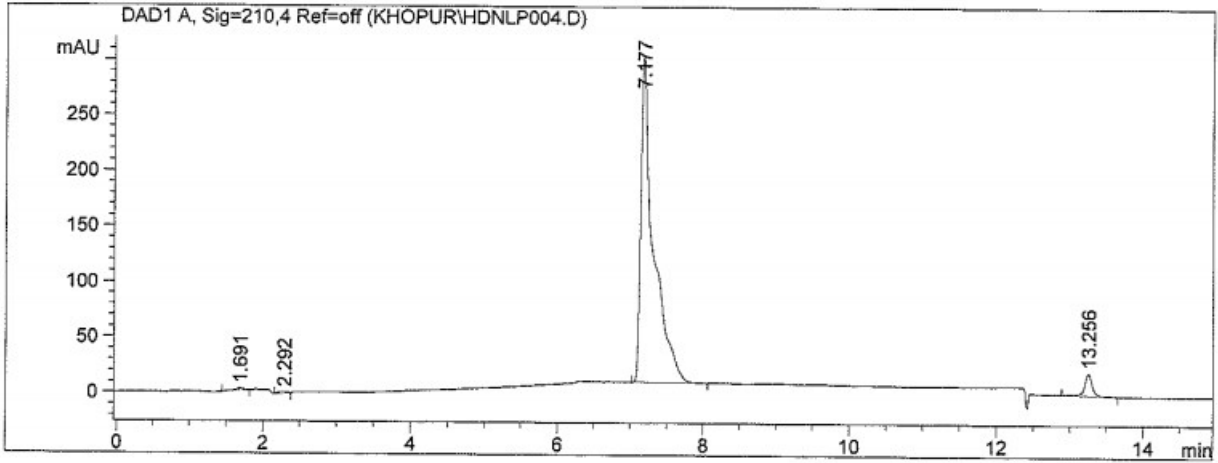


MS



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	N-Rule	e ⁻ Conf
341.1393	1	C ₂₀ H ₂₁ O ₅	100.00	341.1384	-0.9	-2.7	8.4	10.5	ok	even
	2	C ₂₇ H ₁₇	0.06	341.1325	-6.8	-20.0	30.9	19.5	ok	even

HPLC chromatogram



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 Area Percent Report
 =====

Sorted By : Signal
 Calib. Data Modified : 2013/05/28 11:12:51 AM
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

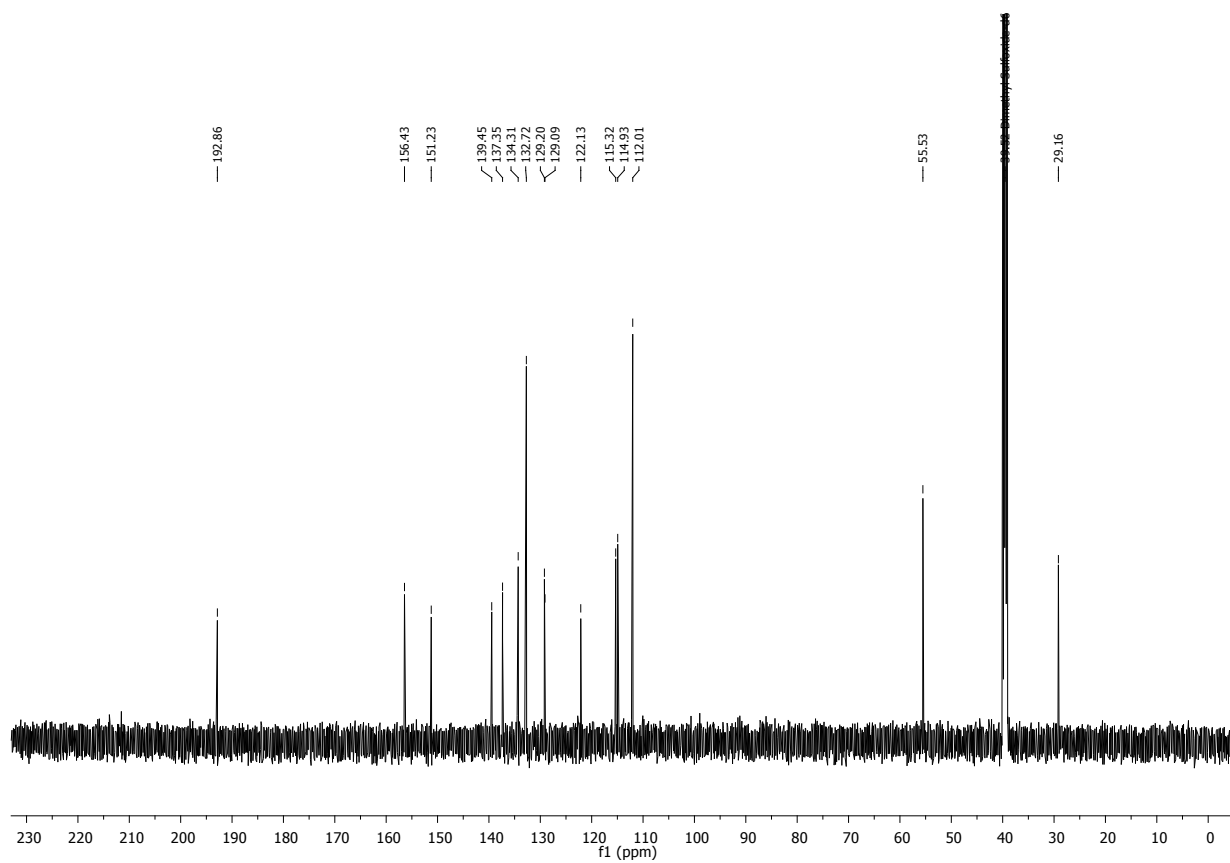
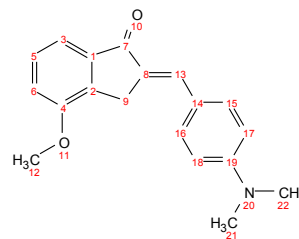
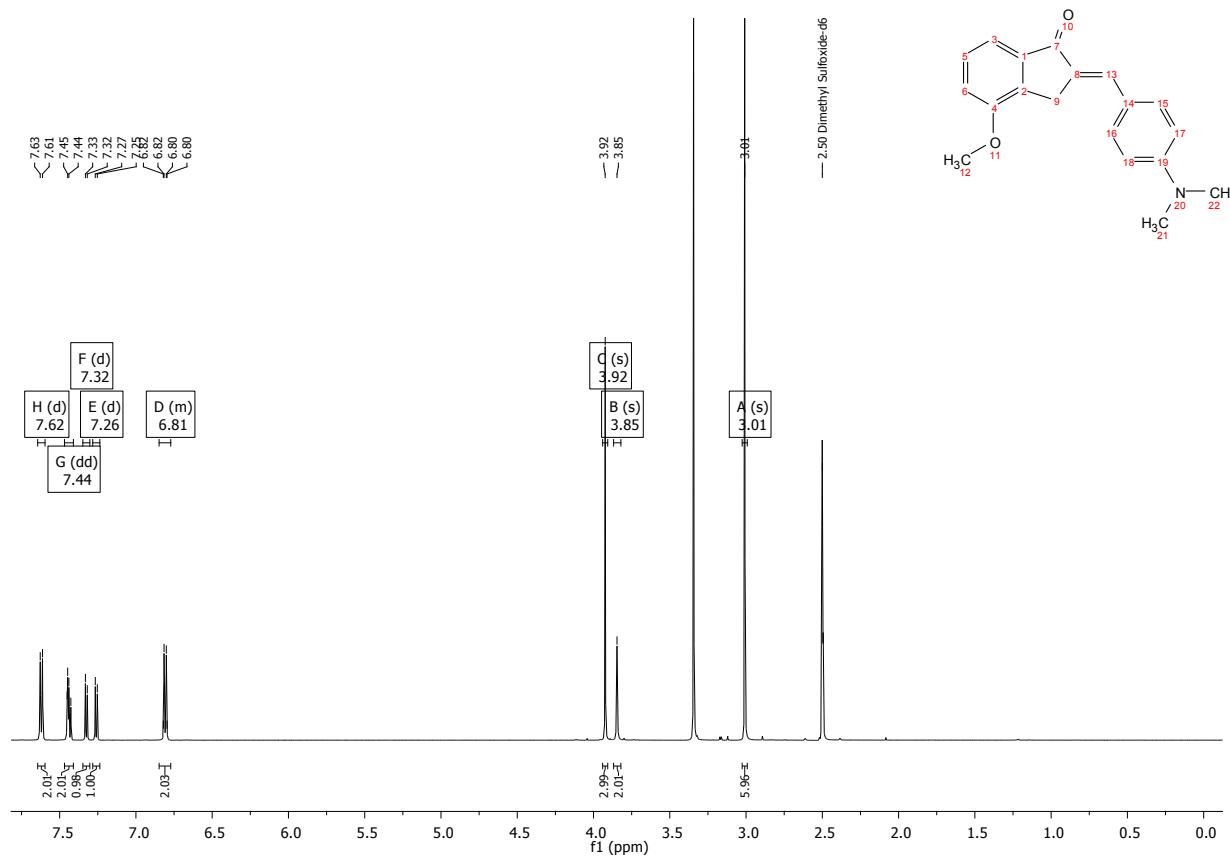
Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.691	BB	0.1315	21.50692	0.5781	?
2	2.292	BB	0.1551	13.59525	0.3654	?
3	2.887		0.0000	0.00000	0.0000	sulf
4	5.220		0.0000	0.00000	0.0000	pir
5	7.177	BB	0.1649	3539.46631	95.1349	?
6	13.256	BBA	0.1086	145.90253	3.9216	?

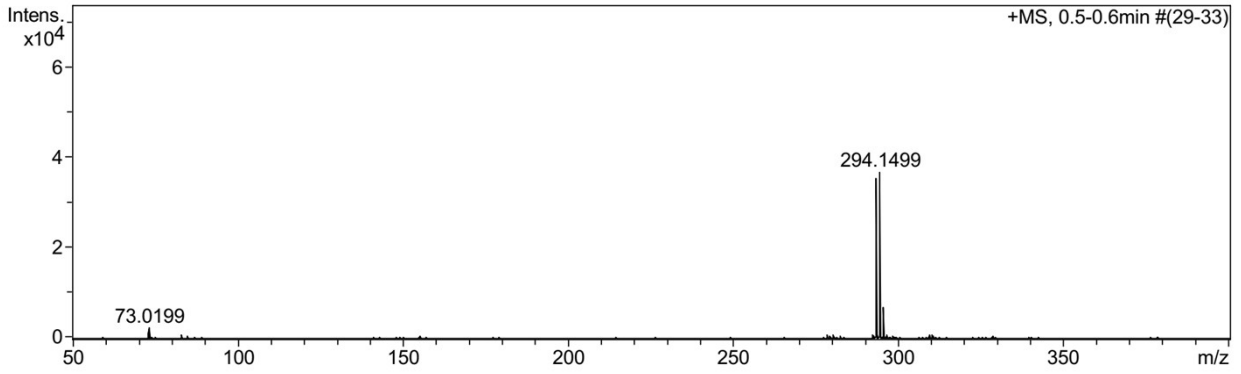
Totals : 3720.47100

(E)-2-(4-(dimethylamino)benzylidene)-4-methoxy-2,3-dihydro-1H-inden-1-one (2g)

NMR spectra

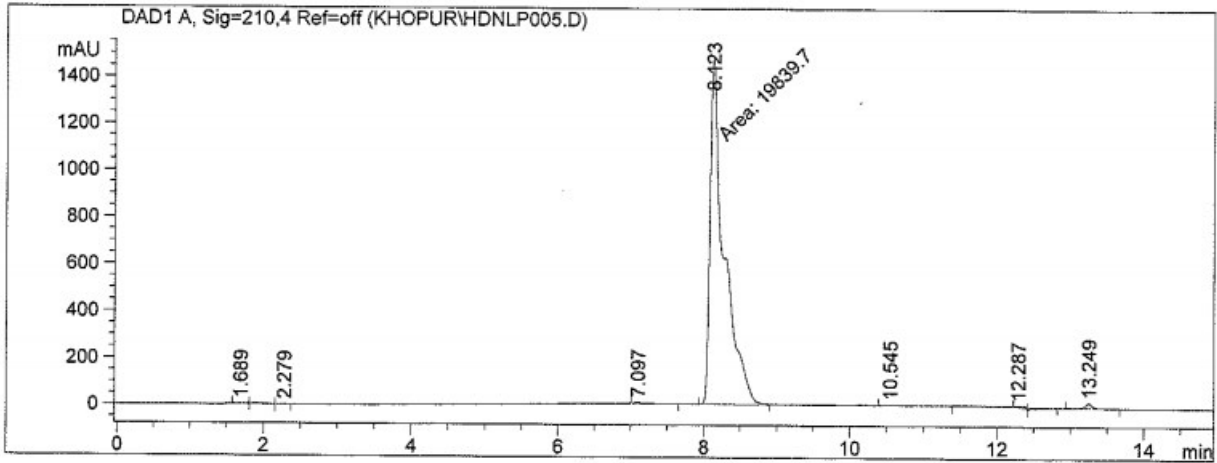


MS



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
293.1432	1	C ₁₉ H ₁₉ N ₂ O ₂	100.00	293.1410	-2.1	-7.3	466.8	11.0	odd	ok
294.1499	1	C ₁₉ H ₂₀ N ₂ O ₂	100.00	294.1489	-1.1	-3.6	12.0	10.5	even	ok

HPLC chromatogram



Area Percent Report

Sorted By : Signal
 Calib. Data Modified : 2013/05/28 11:12:51 AM
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

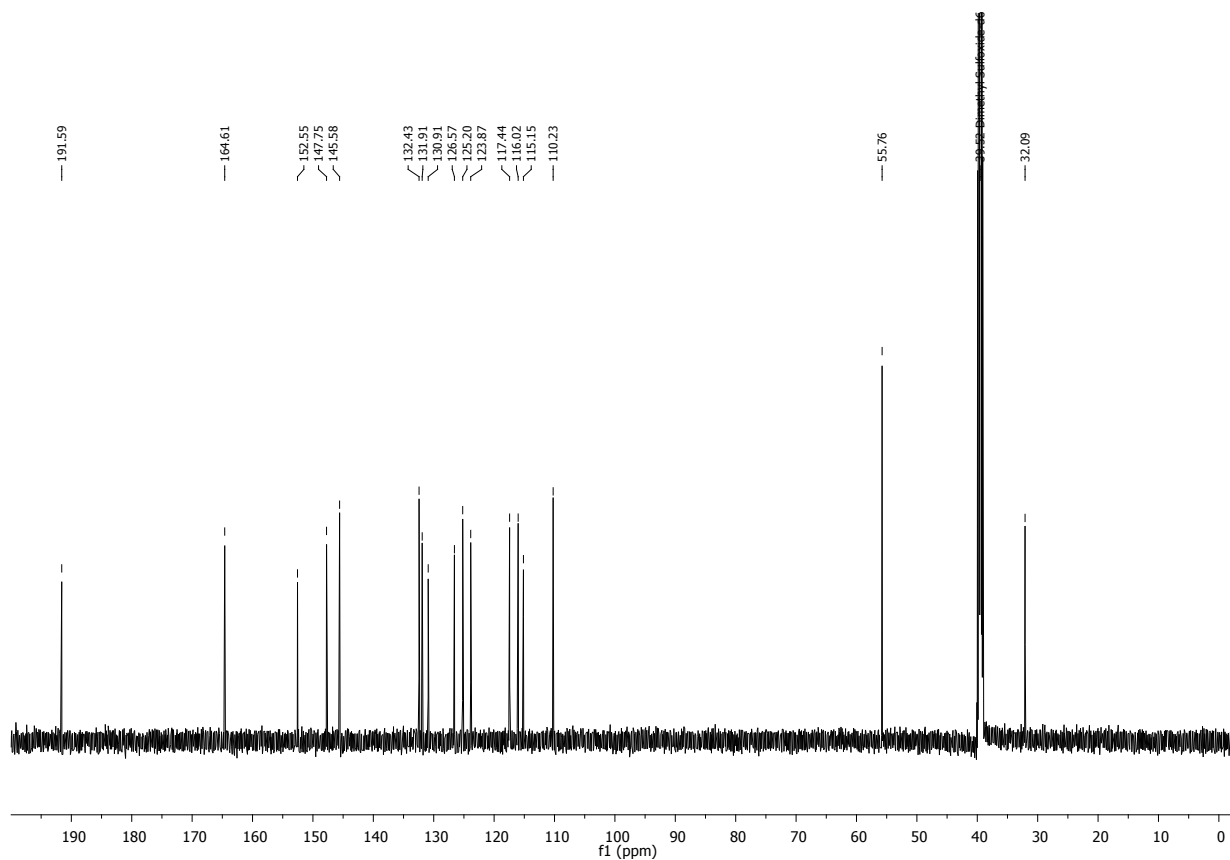
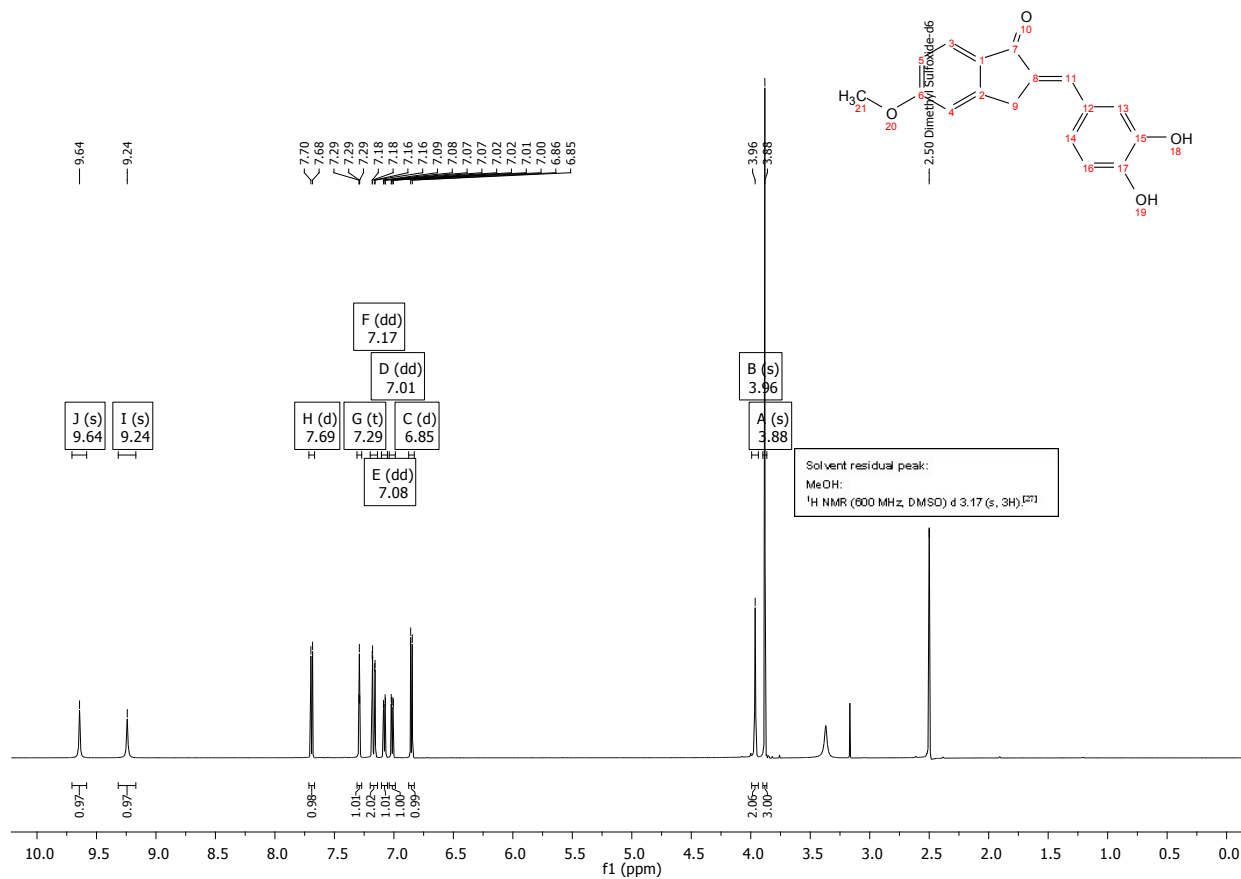
Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.689	BB	0.0762	9.36703	0.0462	?
2	1.912	BB	0.2566	36.69880	0.1811	?
3	2.279	BB	0.1384	13.41213	0.0662	?
4	2.887		0.0000	0.00000	0.0000	sulf
5	5.220		0.0000	0.00000	0.0000	pir
6	7.097	BB	0.1653	49.33882	0.2434	?
7	8.123	MM	0.2245	1.98397e4	97.8861	?
8	10.545	BB	0.2551	20.57146	0.1015	?
9	12.287	BB	0.1766	66.34303	0.3273	?
10	12.466	BB	0.1462	89.51135	0.4416	?
11	13.249	BBA	0.1010	143.20221	0.7065	?

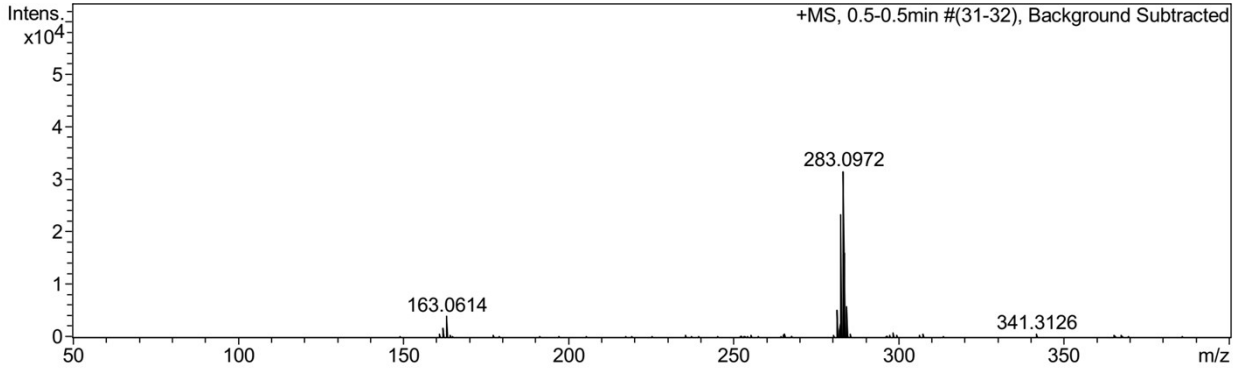
Totals : 2.02681e4

(E)-2-(3,4-dihydroxybenzylidene)-5-methoxy-2,3-dihydro-1H-inden-1-one (2i)

NMR spectra

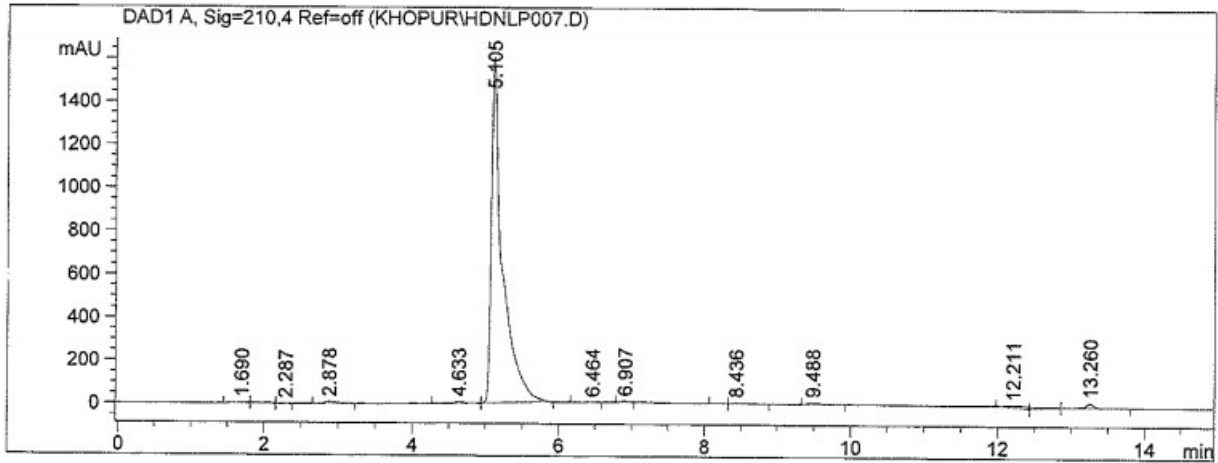


MS



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
283.0972	1	C ₁₇ H ₁₅ O ₄	100.00	283.0965	-0.7	-2.6	3.6	10.5	even	ok

HPLC chromatogram



Area Percent Report

Sorted By : Signal
 Calib. Data Modified : 2013/05/28 11:12:51 AM
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

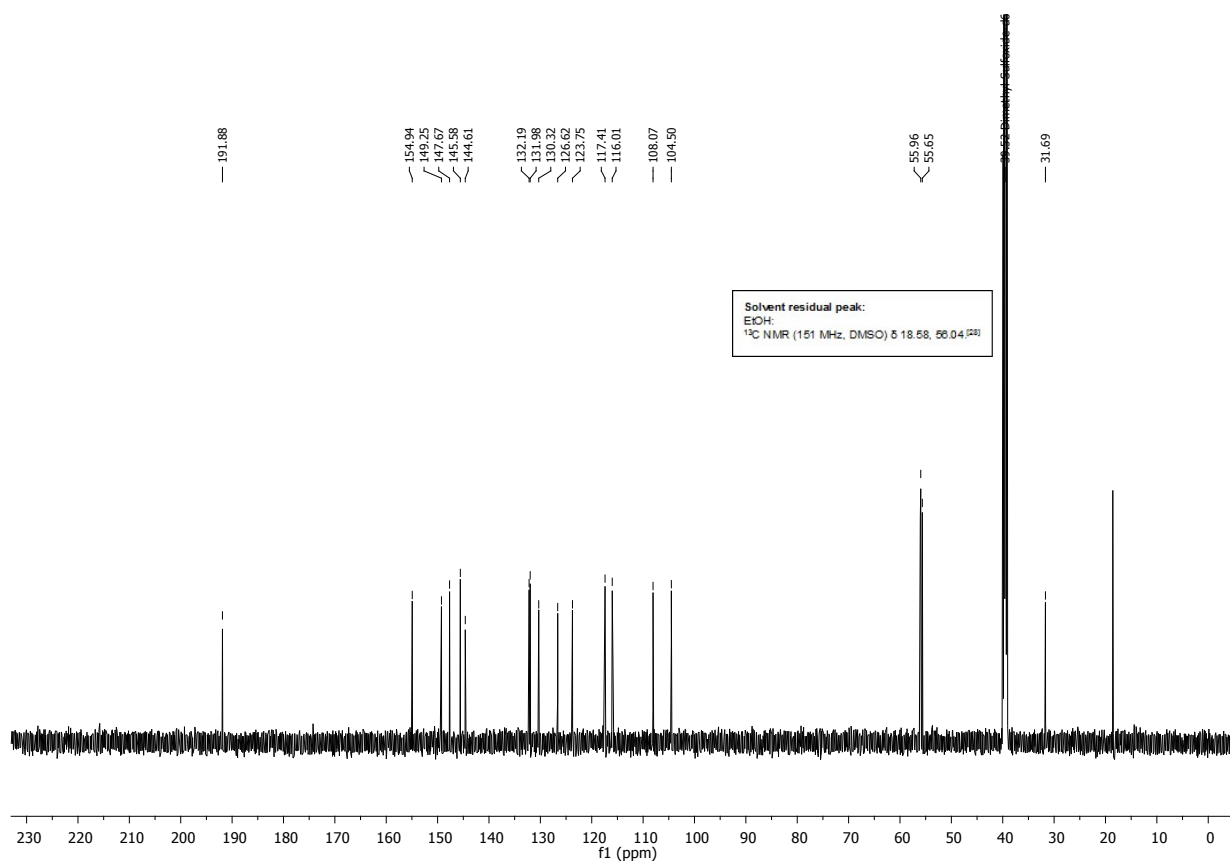
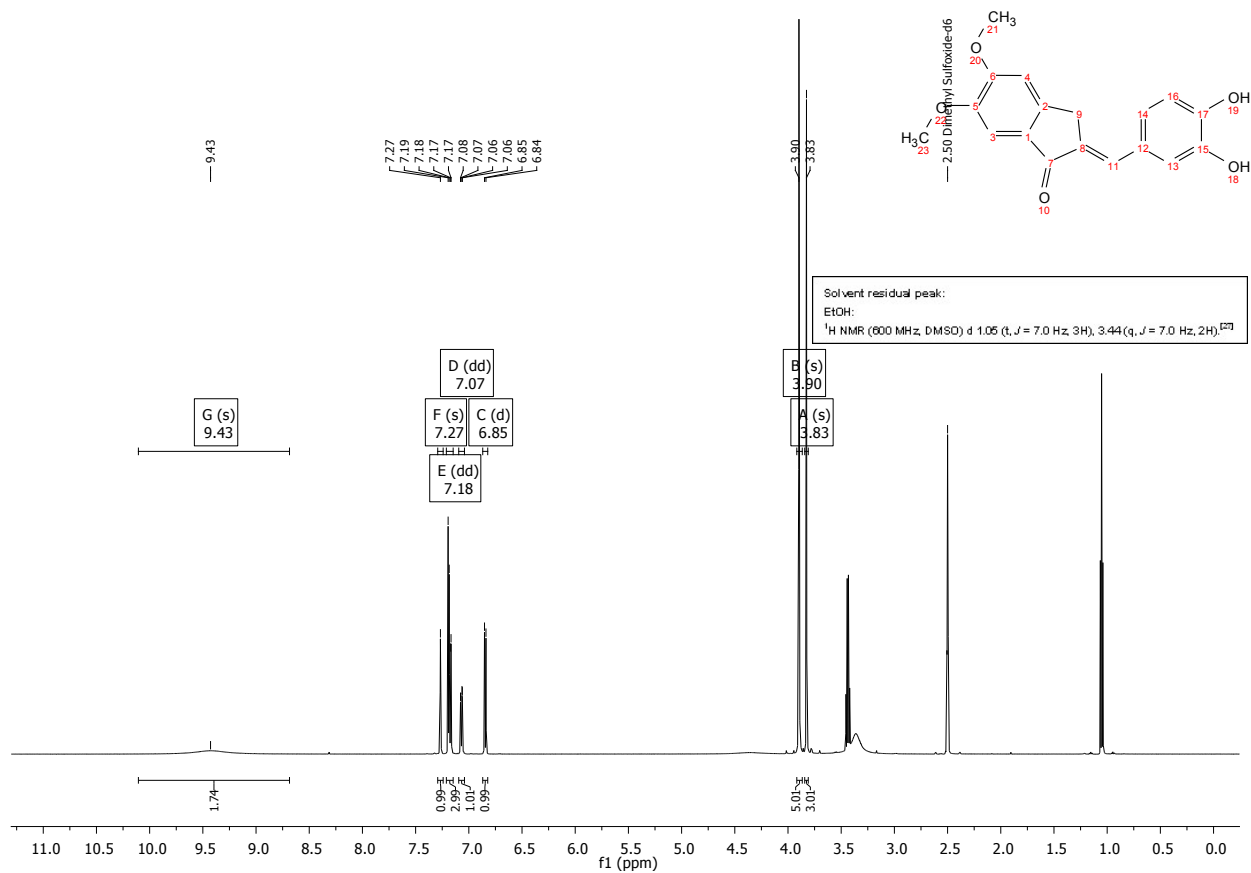
Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.690	BB	0.1166	19.25243	0.1087	?
2	1.909	BB	0.2546	36.24482	0.2047	?
3	2.287	BB	0.1624	14.25192	0.0805	?
4	2.878	BB	0.1429	79.20682	0.4472	sulf
5	4.633	BB	0.1045	53.41726	0.3016	?
6	5.105	BB	0.1448	1.68984e4	95.4186	pir
7	6.464	BB	0.1236	8.95333	0.0506	?
8	6.907	BB	0.1145	33.89564	0.1914	?
9	8.201	BB	0.0984	7.39410	0.0418	?
10	8.436	BB	0.1723	38.94485	0.2199	?
11	9.488	BB	0.1761	75.80923	0.4281	?
12	12.211	BB	0.2860	187.05733	1.0562	?
13	12.476	BB	0.1544	111.31627	0.6286	?
14	13.260	BB	0.1086	145.60353	0.8222	?

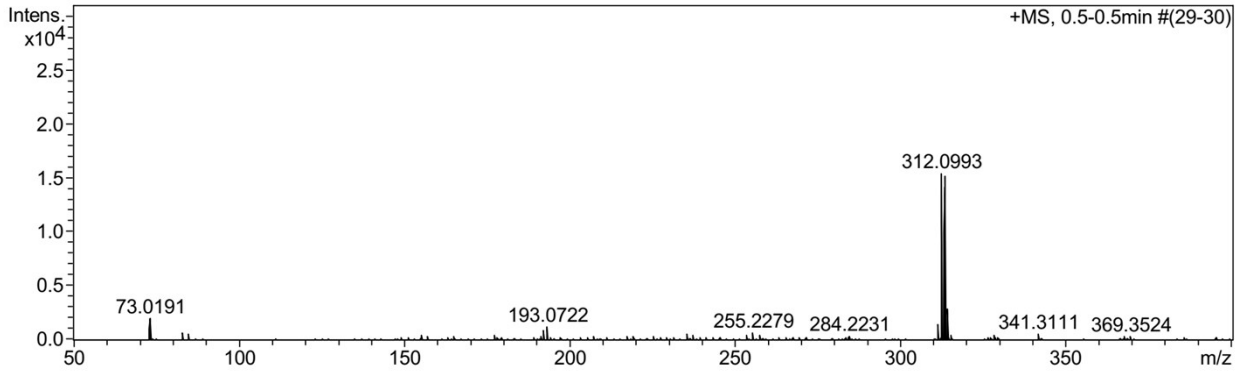
Totals : 1.77098e4

(E)-2-(3,4-dihydroxybenzylidene)-5,6-dimethoxy-2,3-dihydro-1H-inden-1-one (2k)

NMR spectra

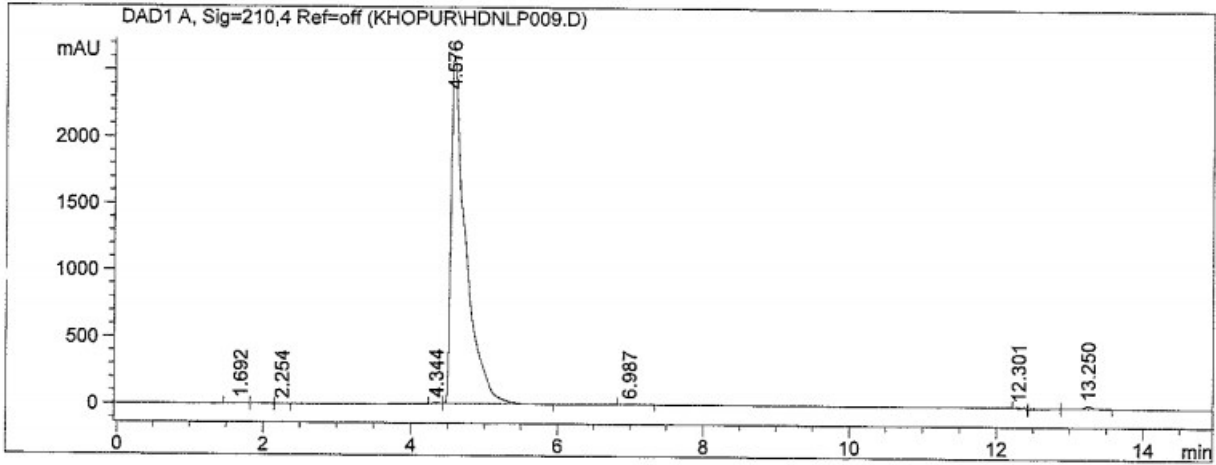


MS



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
312.0993	1	C 18 H 16 O 5	100.00	312.0992	-0.1	-0.2	466.5	11.0	odd	ok
313.1062	1	C 18 H 17 O 5	100.00	313.1071	0.8	2.6	1.1	10.5	even	ok

HPLC chromatogram



Area Percent Report

Sorted By : Signal
 Calib. Data Modified : 2013/05/28 11:12:51 AM
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

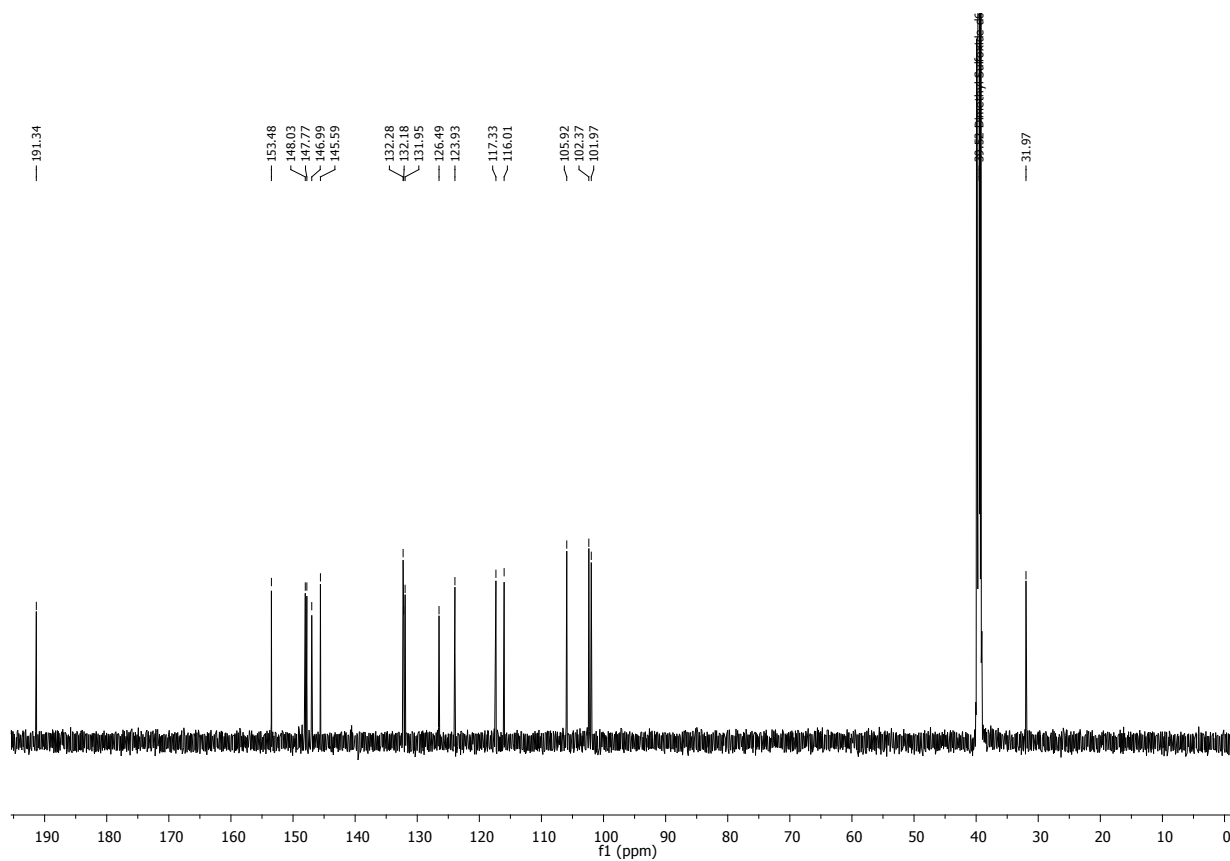
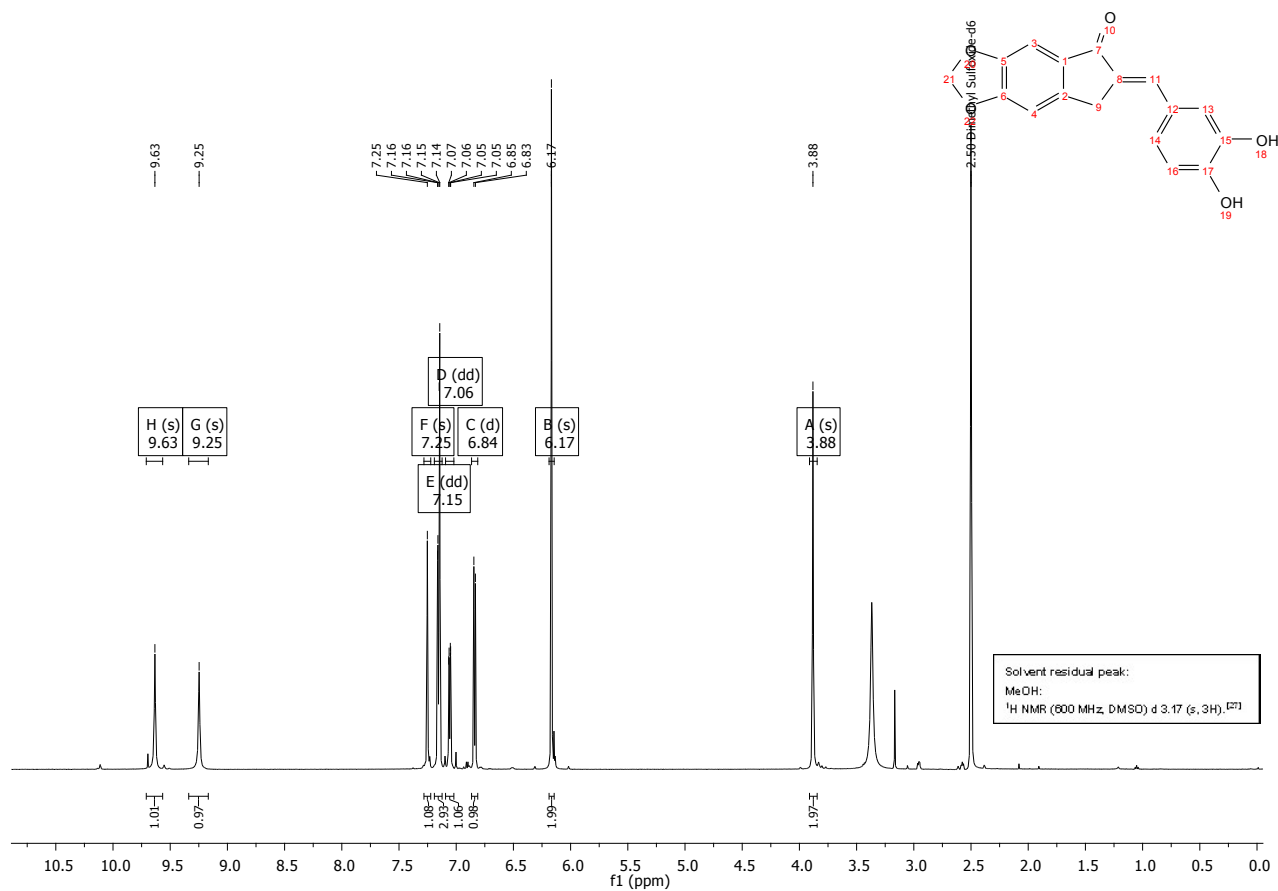
Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.692	BB	0.1261	21.17537	0.0584	?
2	1.904	BB	0.2664	31.88166	0.0879	?
3	2.254	BB	0.1301	12.89552	0.0356	?
4	2.887		0.0000	0.00000	0.0000	sulf
5	4.344	BB	0.0775	38.15683	0.1052	?
6	4.576	BB	0.1908	3.57547e4	98.5685	?
7	5.220		0.0000	0.00000	0.0000	pir
8	6.987	BB	0.1403	41.22489	0.1136	?
9	12.301	BB	0.1567	83.84877	0.2312	?
10	12.473	BB	0.1642	143.97931	0.3969	?
11	13.250	BB	0.0979	146.10318	0.4028	?

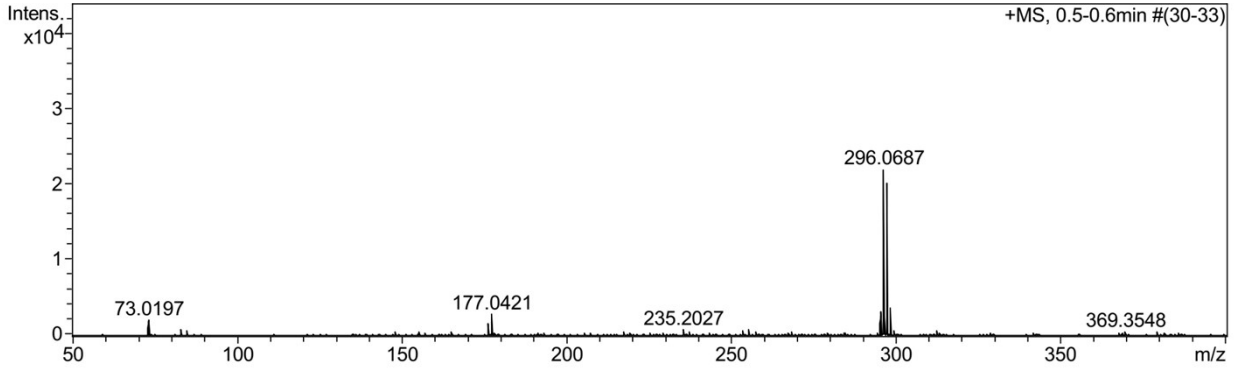
Totals : 3.62740e4

(E)-6-(3,4-dihydroxybenzylidene)-6,7-dihydro-5H-indeno[5,6-d][1,3]dioxol-5-one (2m)

NMR spectra

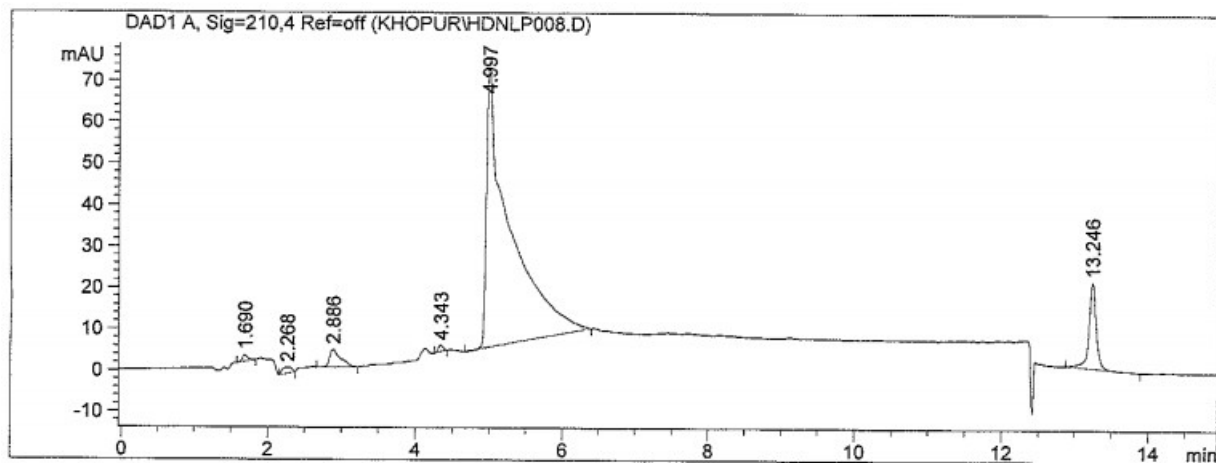


MS



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
296.0687	1	C ₁₇ H ₁₂ O ₅	100.00	296.0679	-0.7	-2.5	430.4	12.0	odd	ok
297.0755	1	C ₁₇ H ₁₃ O ₅	100.00	297.0757	0.3	0.9	1.8	11.5	even	ok

HPLC chromatogram



Area Percent Report

Sorted By : Signal
Calib. Data Modified : 2013/05/28 11:12:51 AM
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.690	BB	0.0814	8.84966	0.5128	?
2	2.268	BB	0.1558	13.83012	0.8014	?
3	2.886	BB	0.1452	45.37901	2.6297	sulf
4	4.343	BB	0.0727	6.92007	0.4010	?
5	4.997	BB	0.2767	1504.45593	87.1811	?
6	5.220		0.0000	0.00000	0.0000	pir
7	13.246	BB	0.1060	146.23259	8.4740	?

Totals : 1725.66738

Notes and references

27 H.E. Gottlieb, V. Kotlyar, A. Nudelman, *J. Org. Chem.*, 1997, **62**,7512-7515