Electronic Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

Direct *anti* and *regio*-specific *aldol* reactions of cyclododecanone catalyzed by Alkali metal hydroxides: Implications for supramolecular helical design

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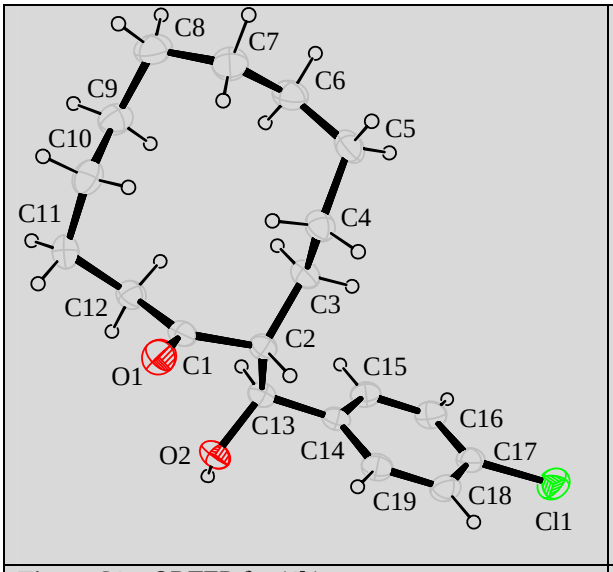


Figure S1a. ORTEP for **(4h)**

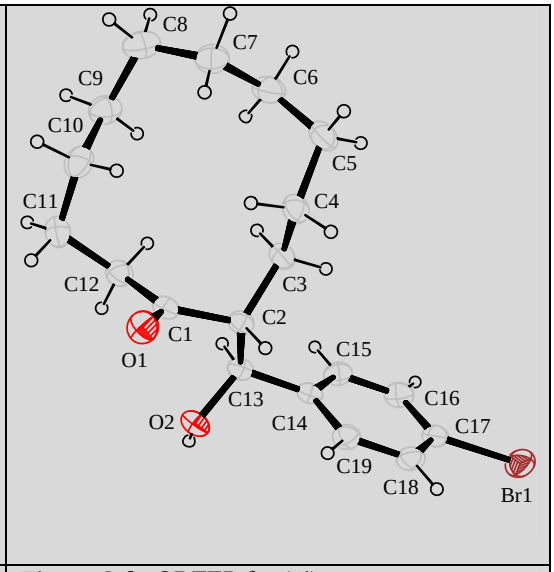


Figure S1b. ORTEP for **(4i)**

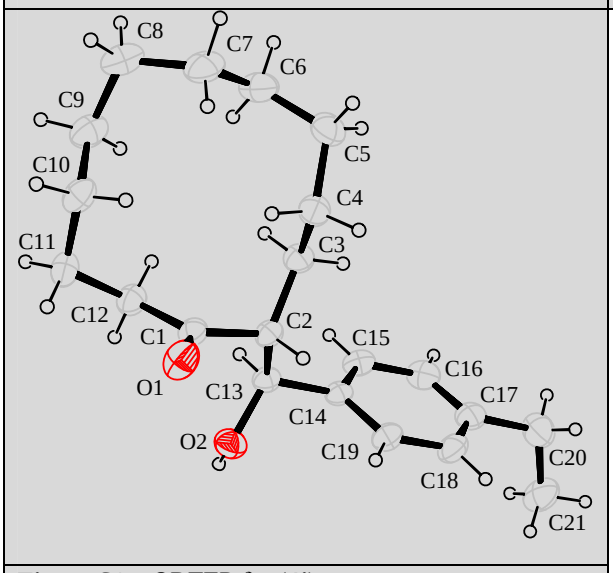


Figure S1a. ORTEP for **(4j)**

Figure S1. A view of **4h-j** with non-H atoms shown as probability ellipsoids at 30% levels drawn with ORTEP (Farrugia, 1997). H atoms radii are on an arbitrary scale.

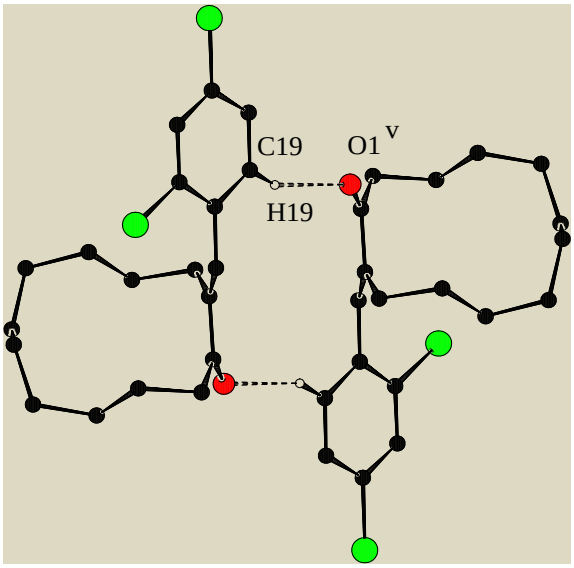
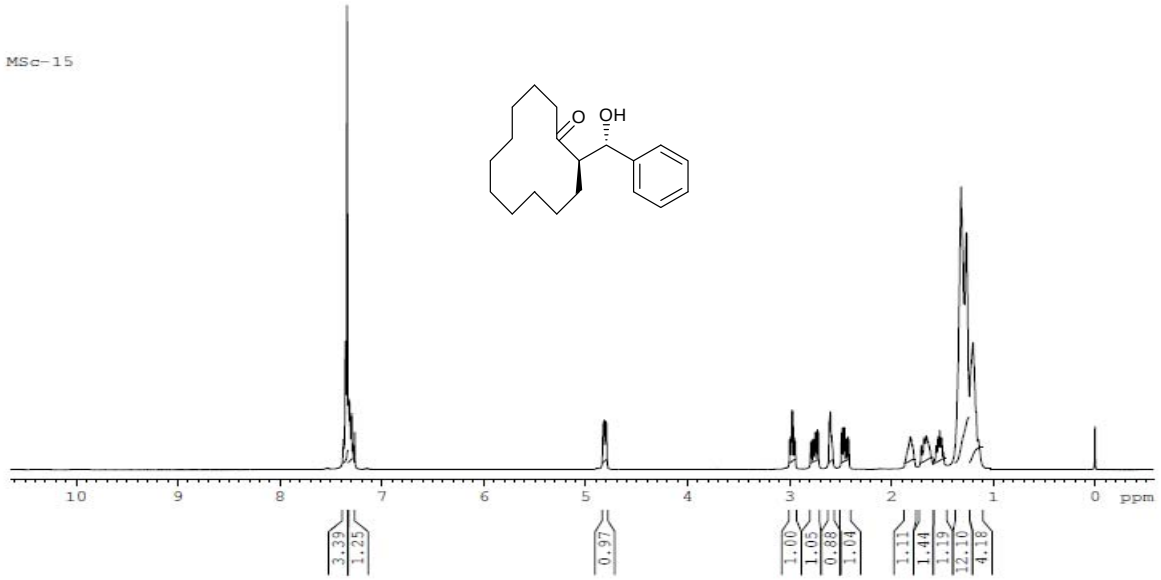


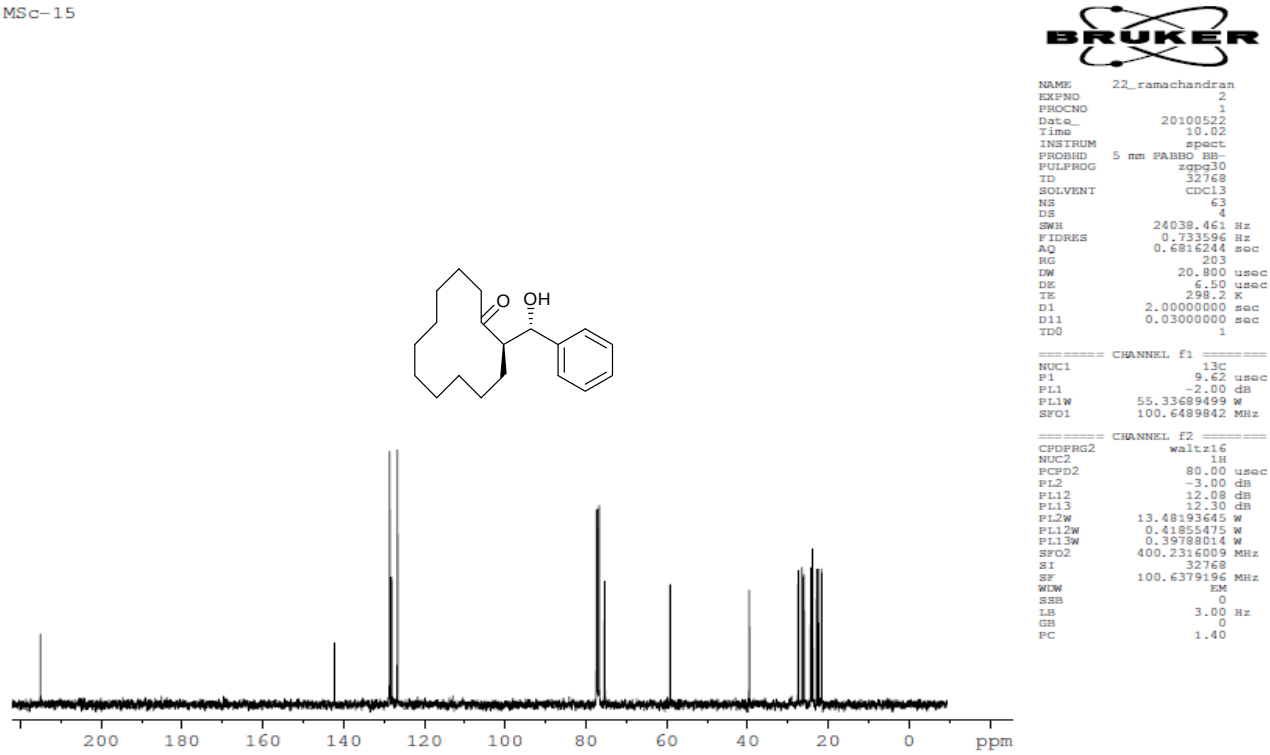
Figure S2. C-H…O linked molecular dimers in **5c.**

NMR spectra / HPLC data:

^{1}HNMR of compound (4a):



C^{13}NMR of compound (4a):



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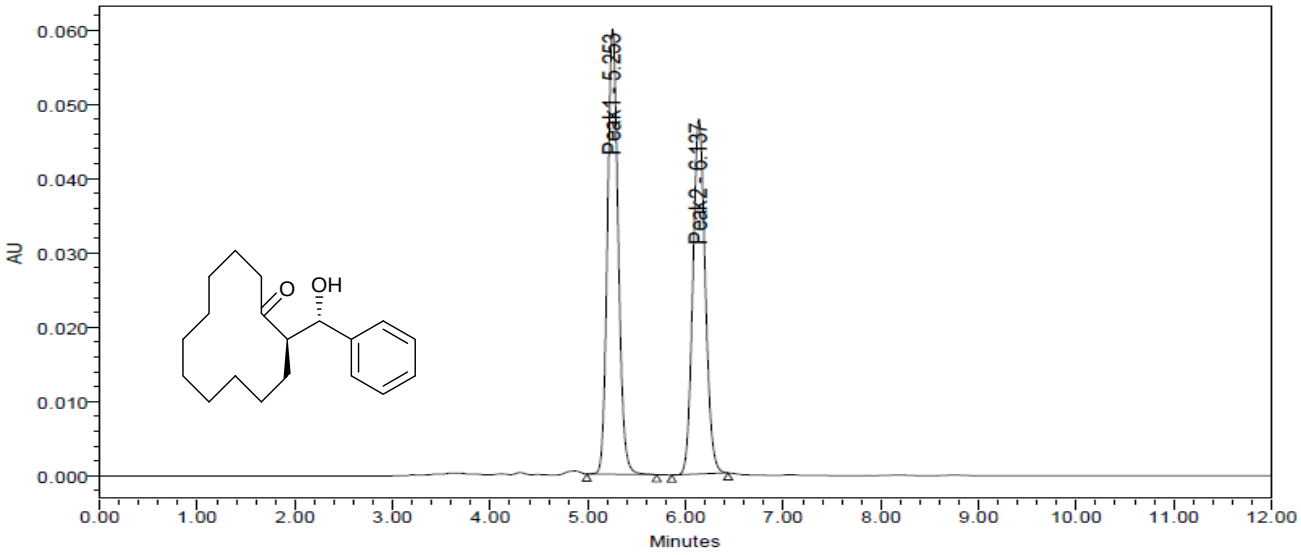

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1	Peak1	5.253	Found	458539	52.04	59885	55.64	Bb	4.585e+005	Q20	214
2	Peak2	6.137	Found	422621	47.96	47745	44.36	Bb	4.226e+005	Q20	173

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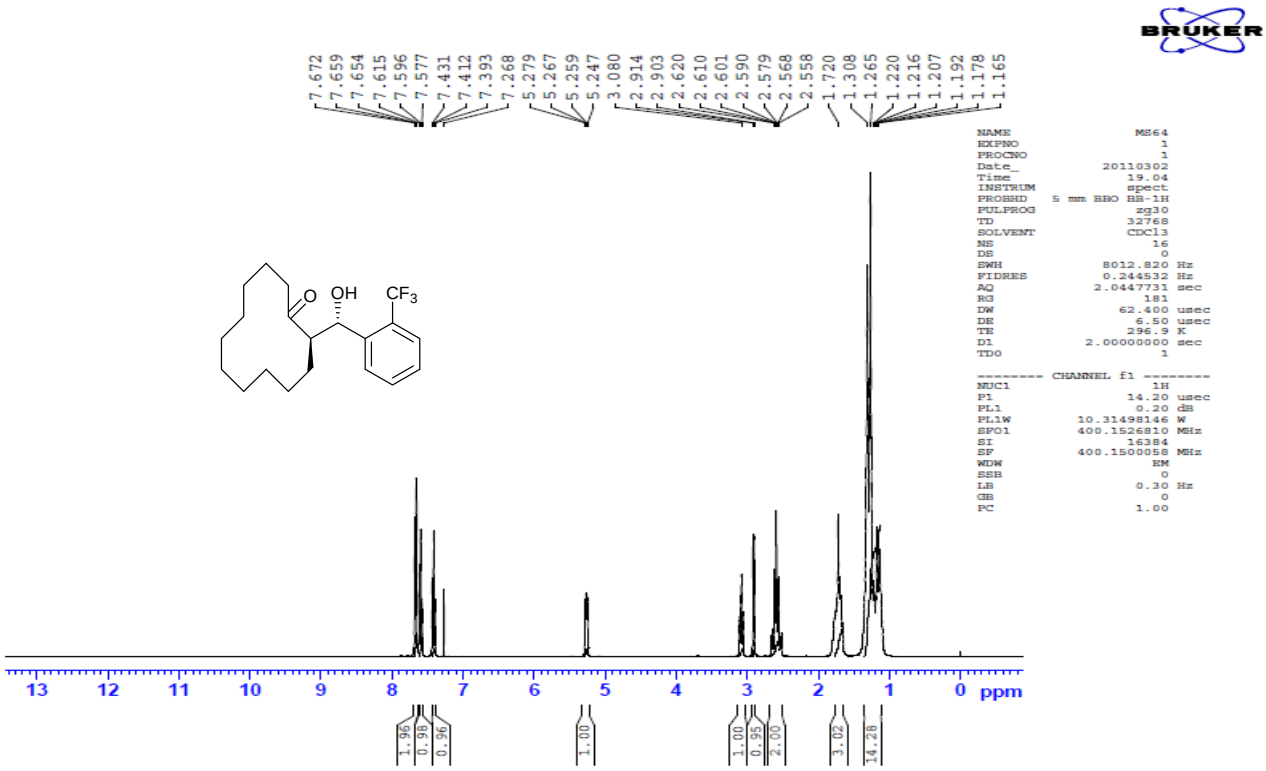

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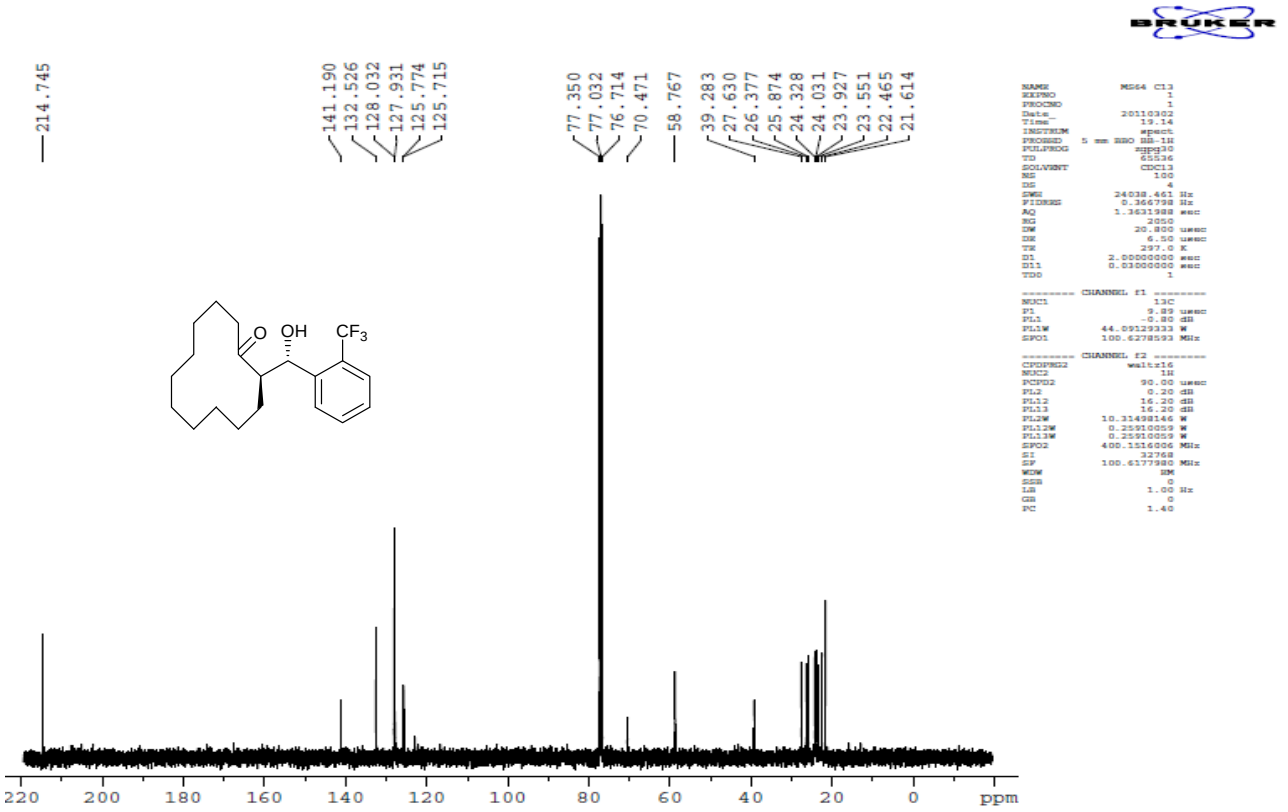

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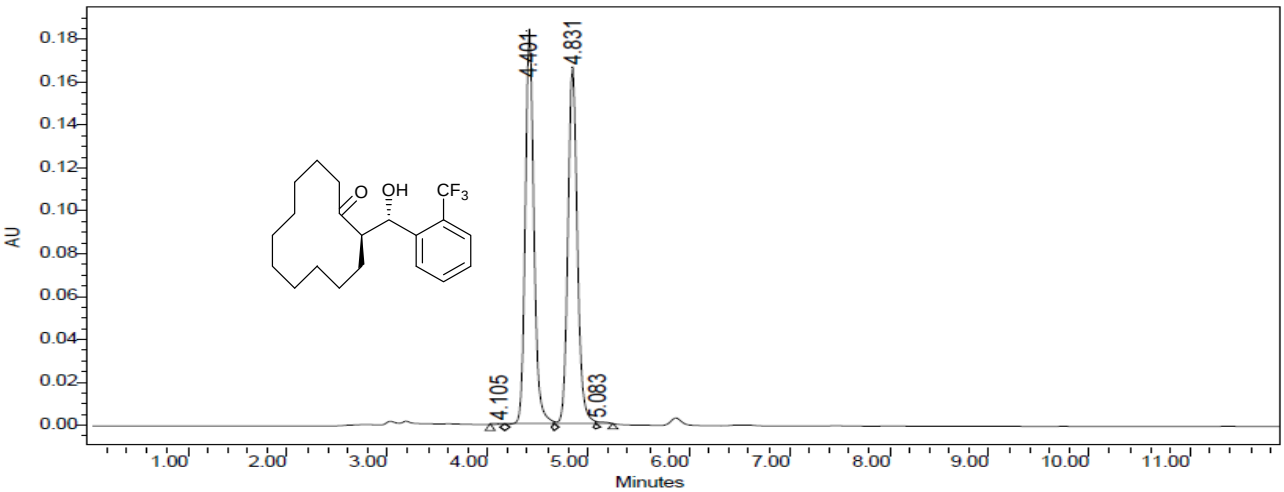
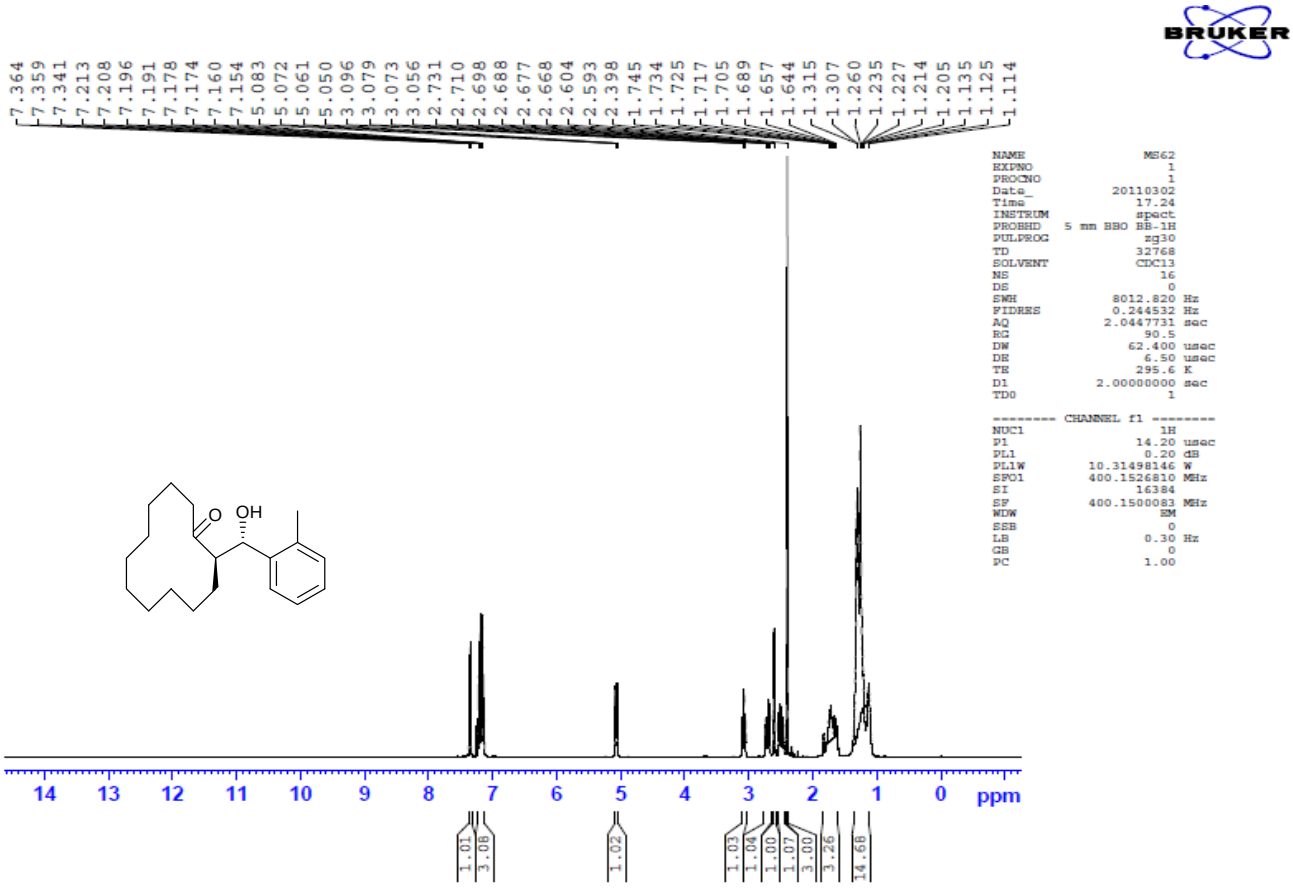


	RT (min)	Area (µV*sec)	% Area	Height (µV)	% Height
1	4.105	752	0.03	171	0.05
2	4.401	1104538	50.09	183000	52.22
3	4.831	1092920	49.57	166233	47.43
4	5.083	6773	0.31	1059	0.30

^{1}H NMR of compound (4c)



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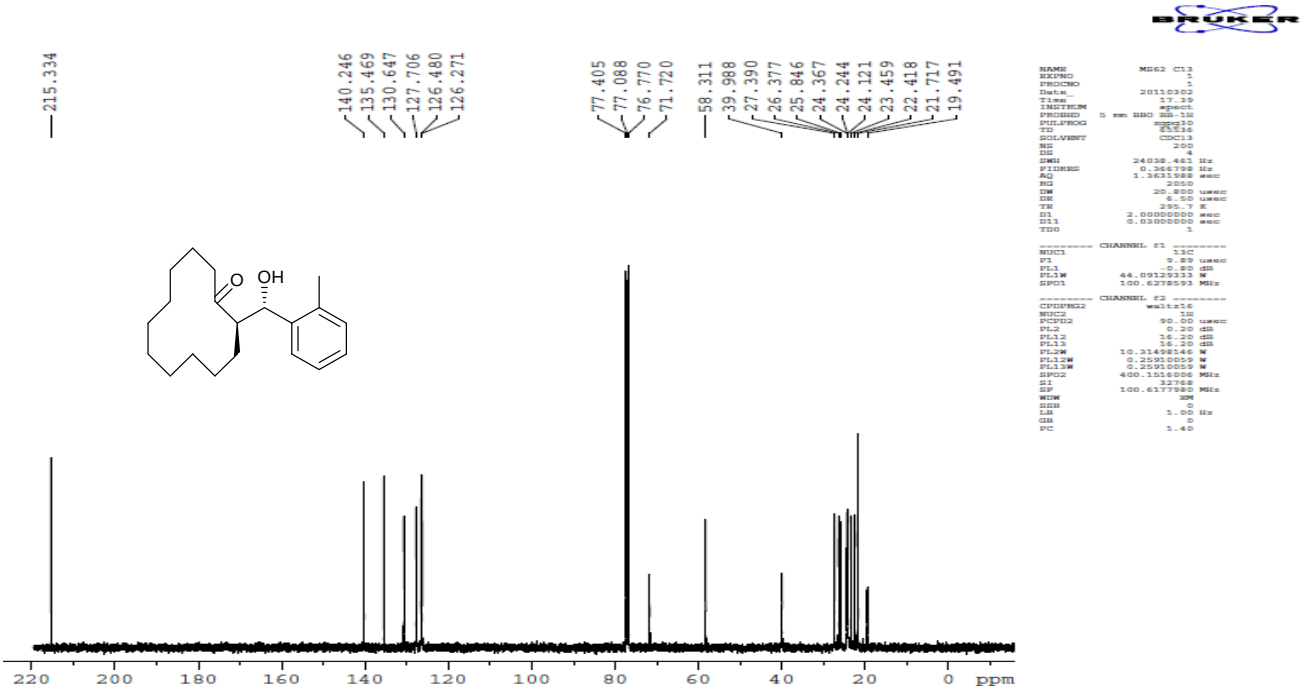

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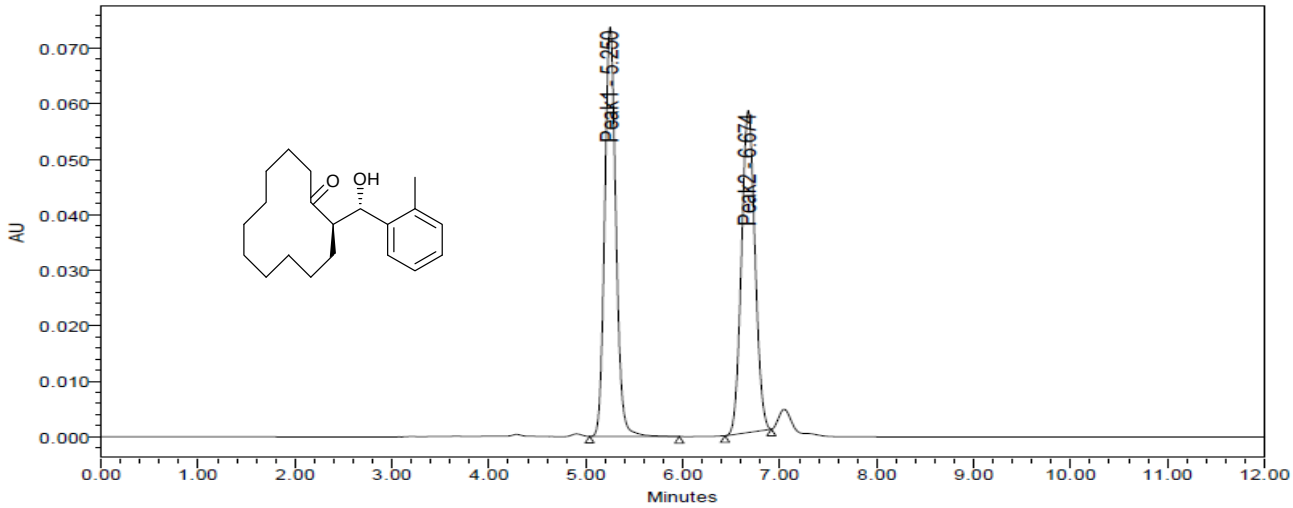

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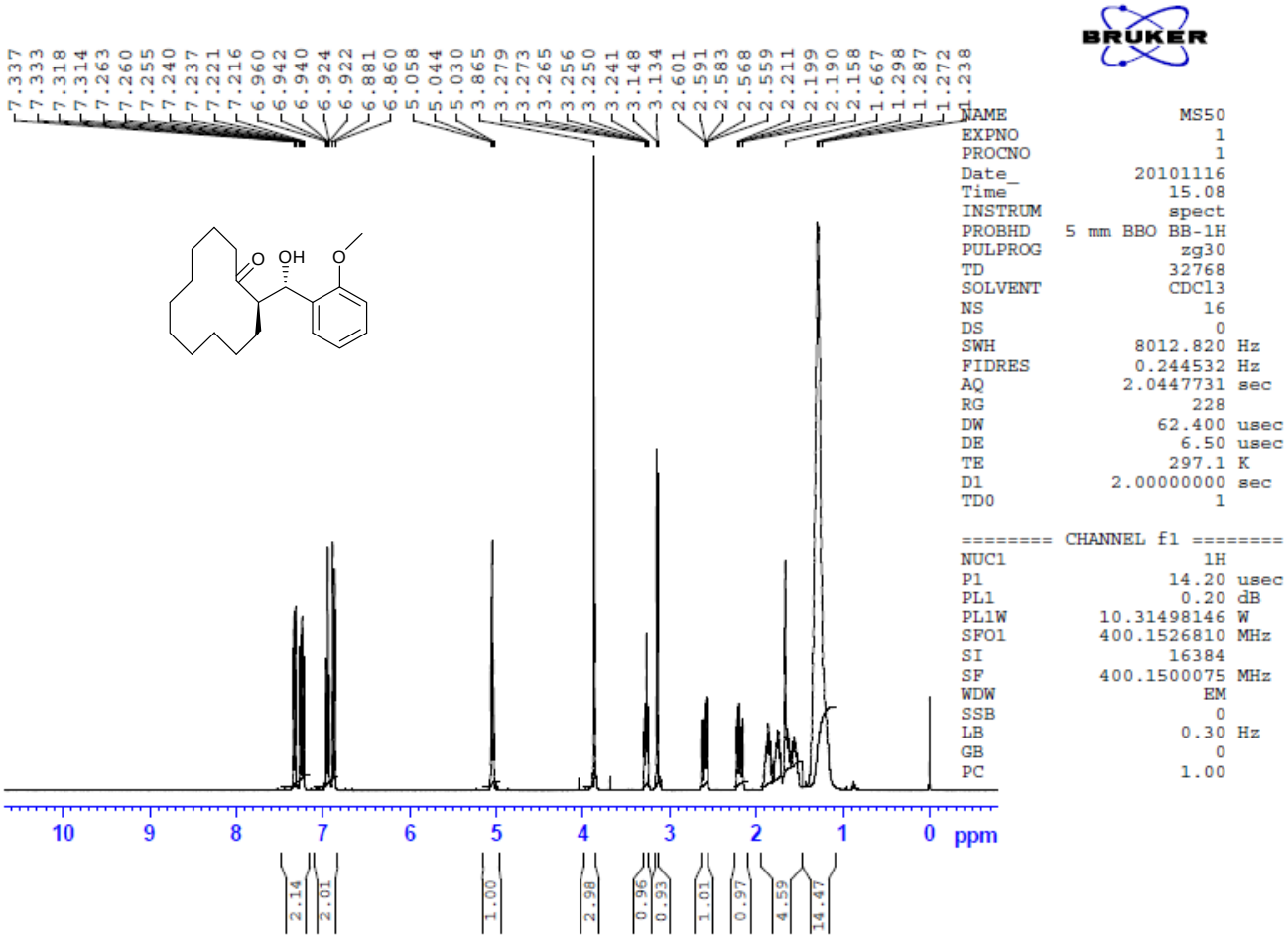
1	Peak1	5.250	Found	594684	51.30	73791	55.98	BB	5.947e+005	Q20	277
2	Peak2	6.674	Found	564512	48.70	58026	44.02	BB	5.645e+005	Q20	143

^{1}H NMR of compound (4d)



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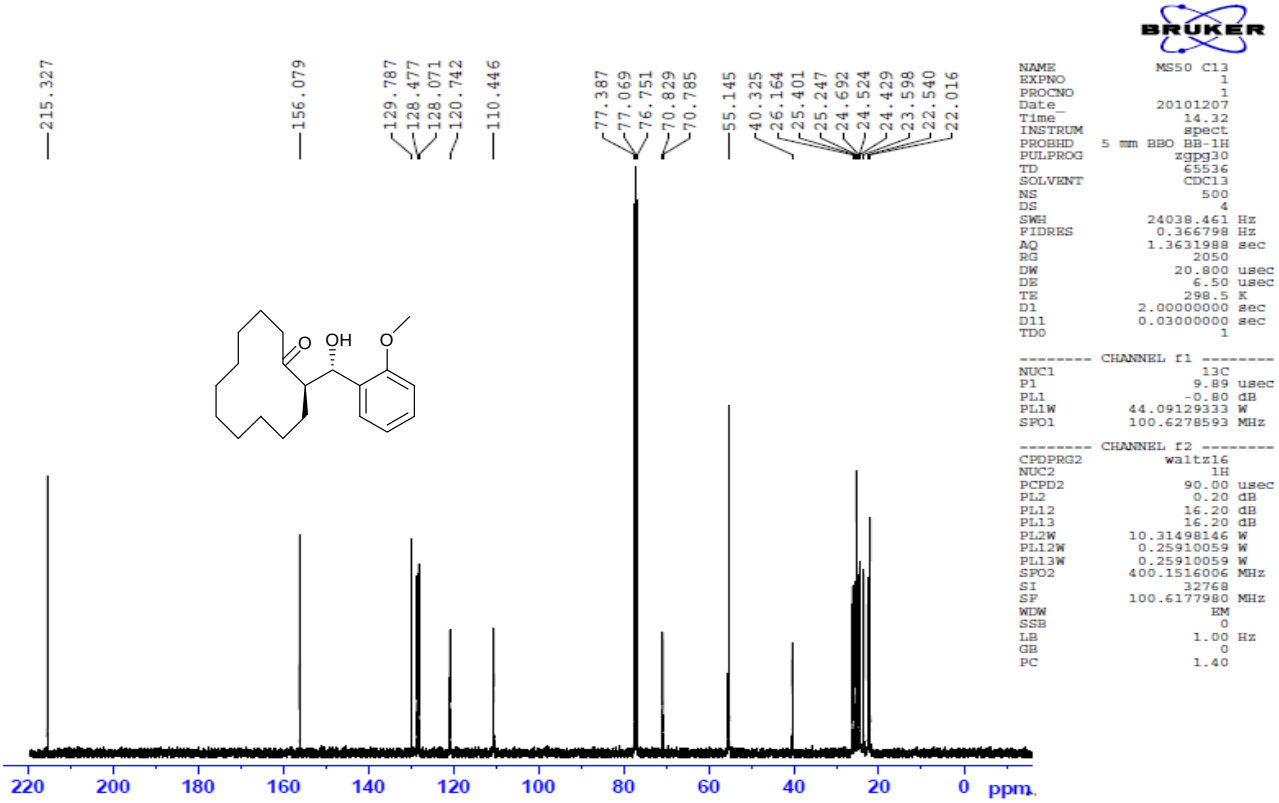

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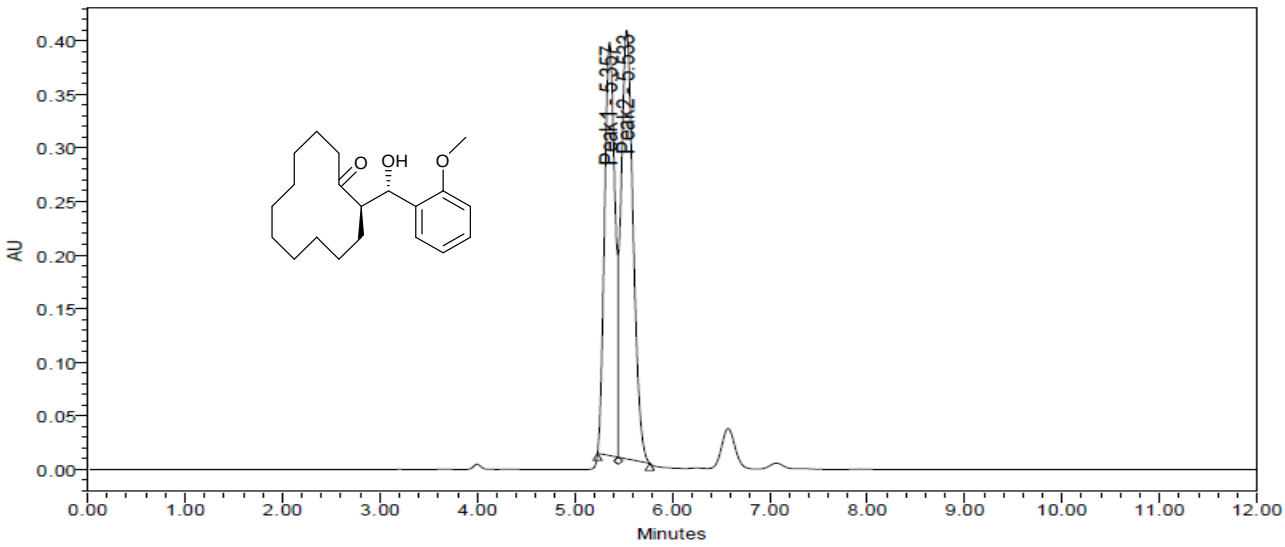

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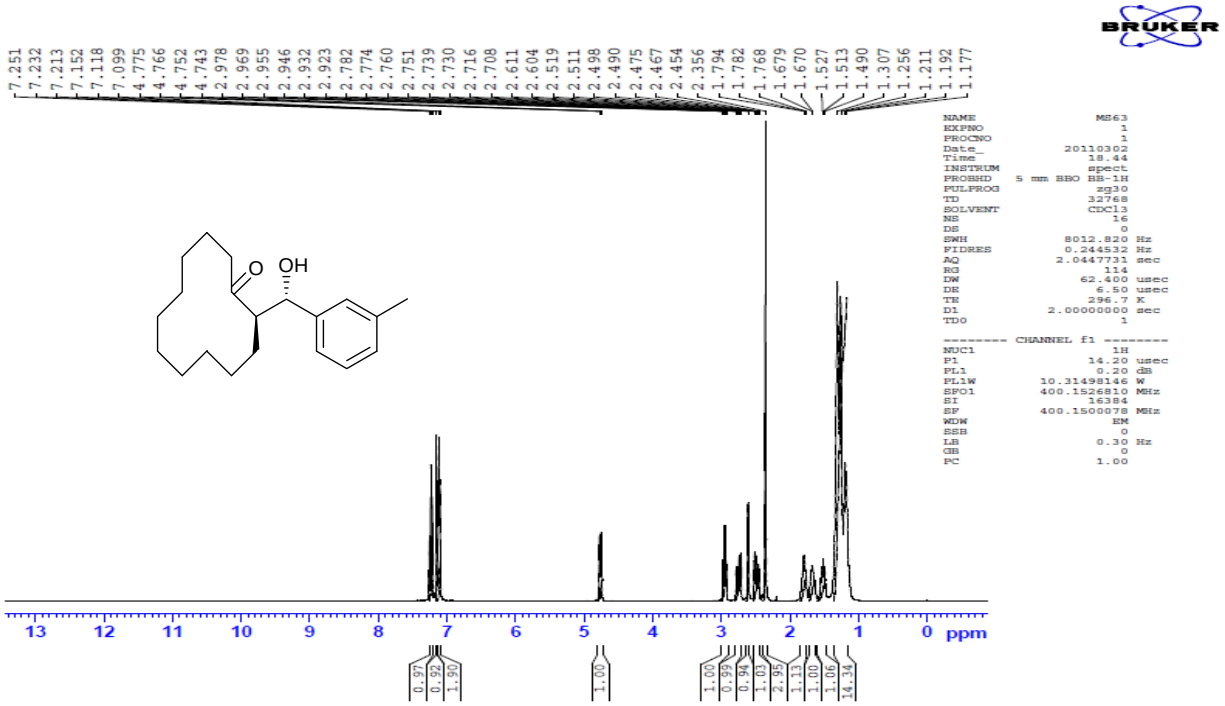
^{1}HNMR of compound (4e)



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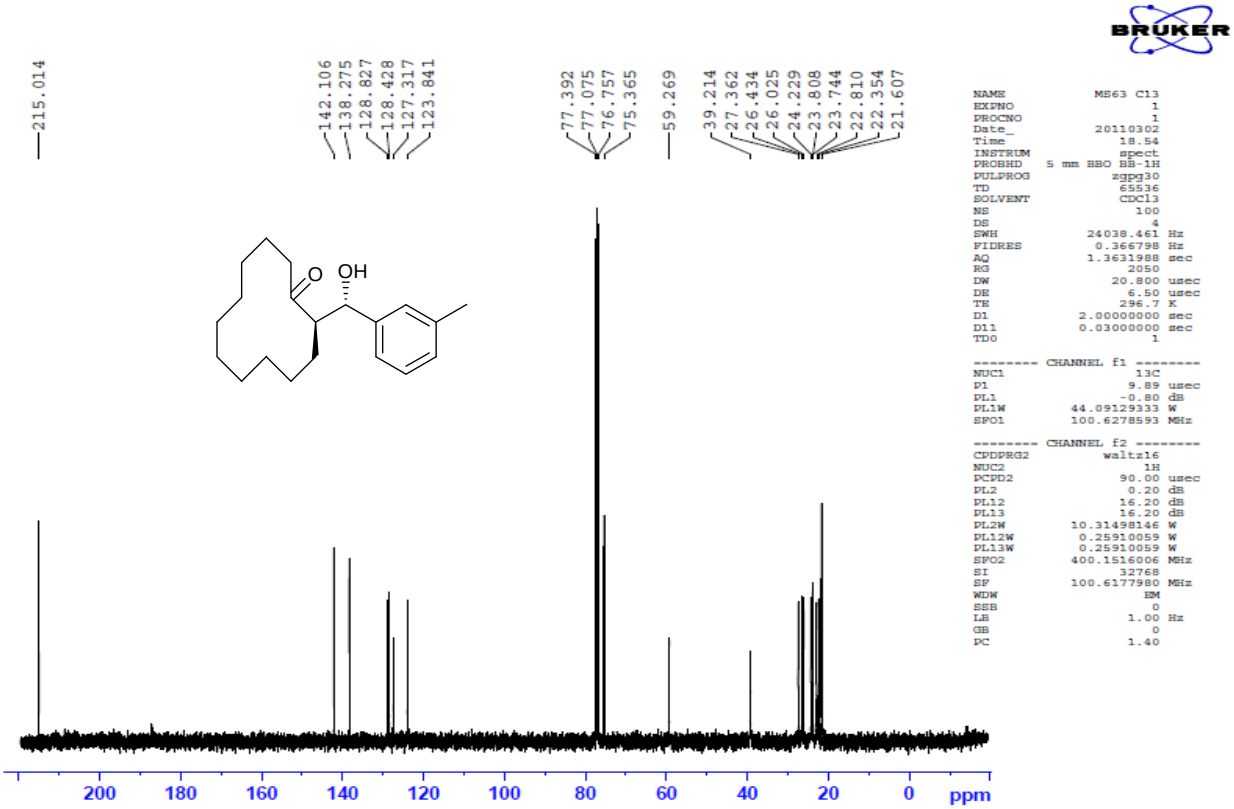

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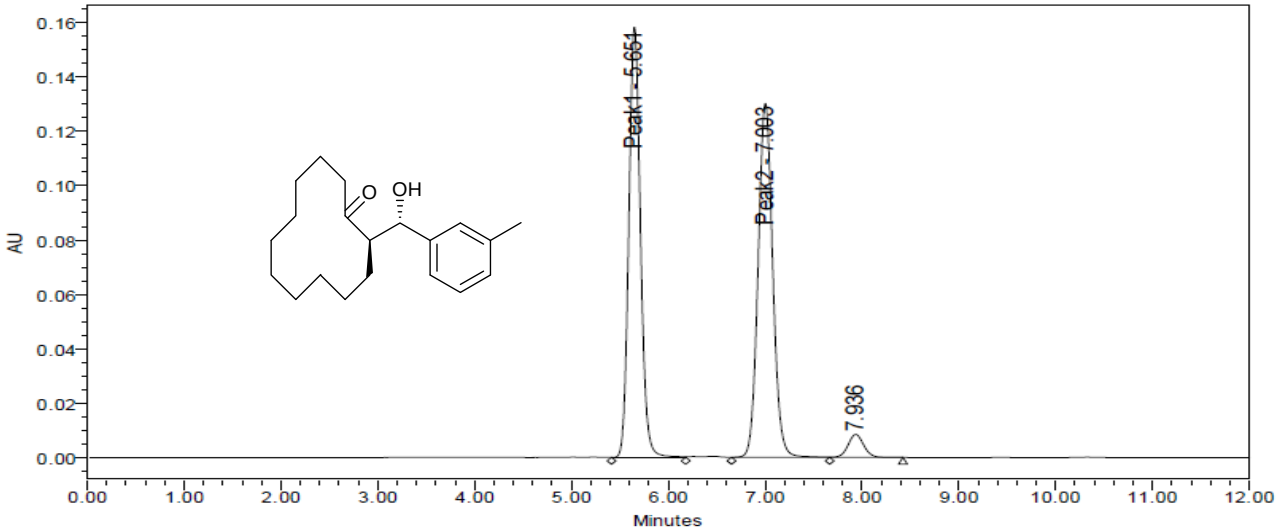

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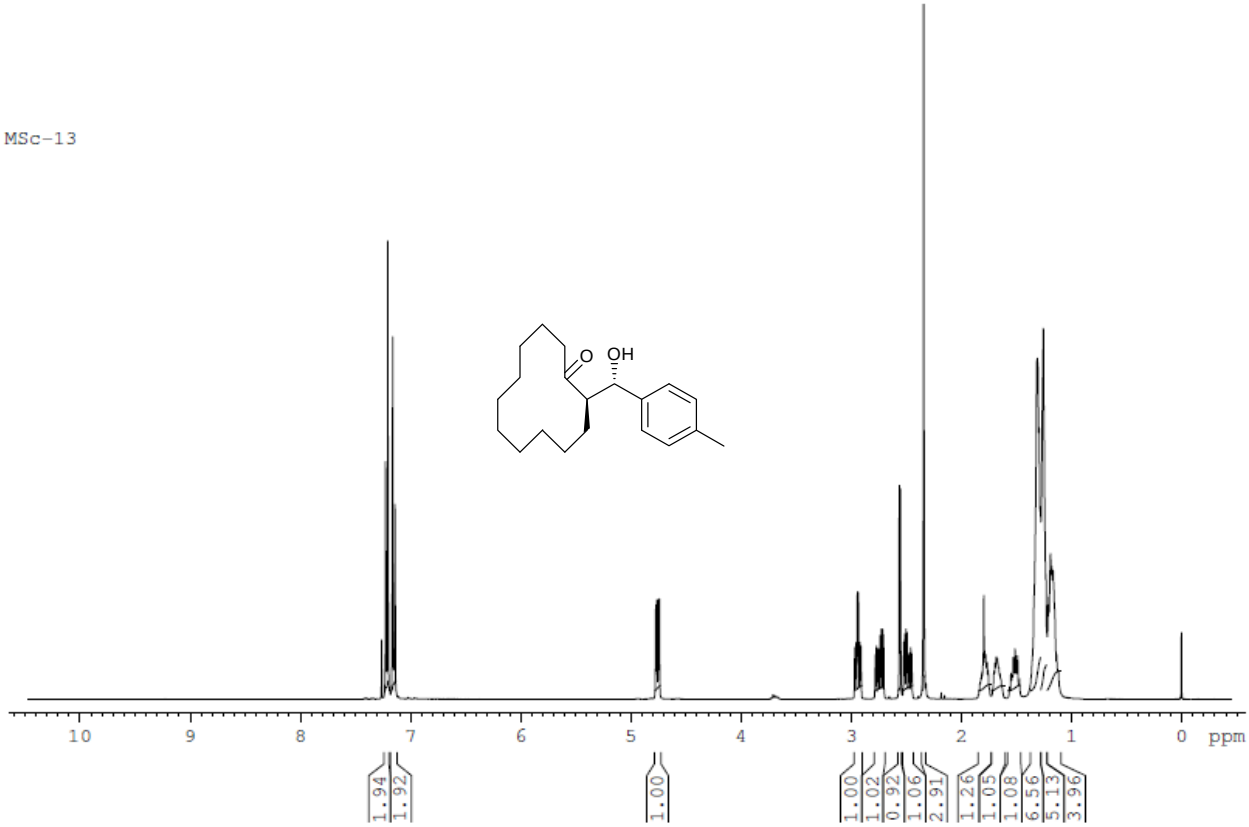
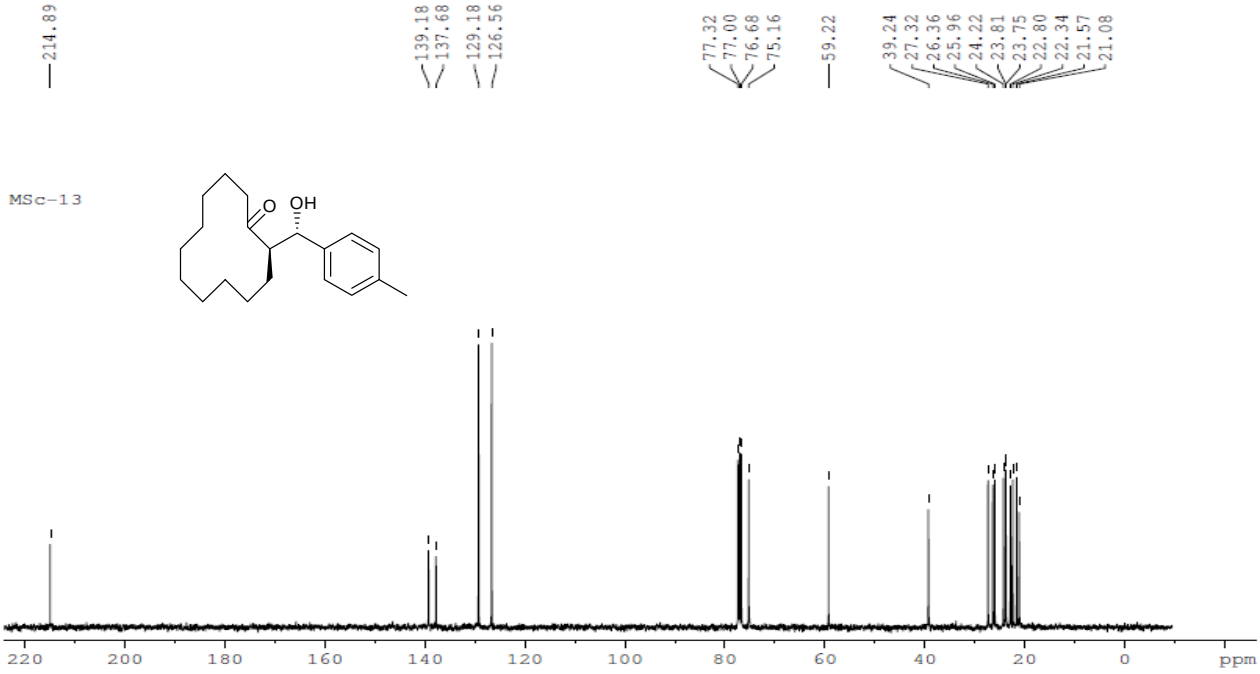
2	Peak2	7.003	Found	1369795	49.08	130274	43.86	VV	1.370e+006	Q20
3		7.936	Unknown	95295	3.41	8477	2.85	VB		

^{1}H NMR of compound (4f)



C^{13} NMR of compound (4f)



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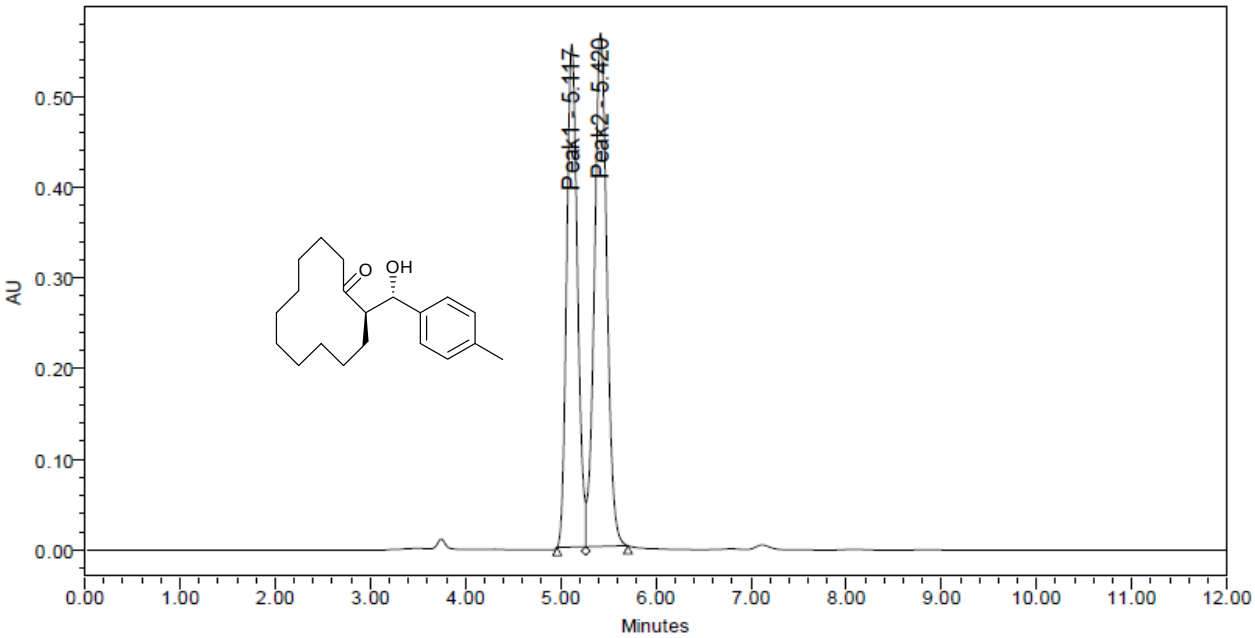

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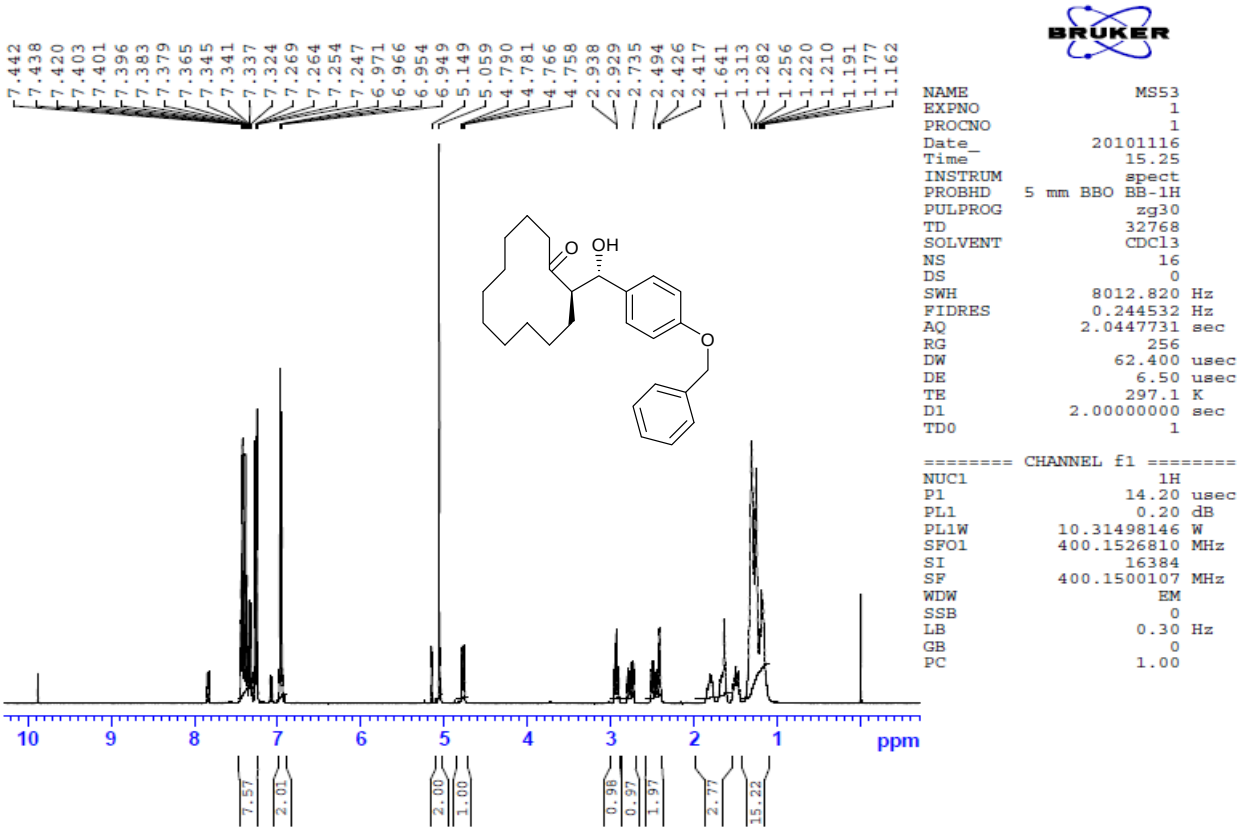
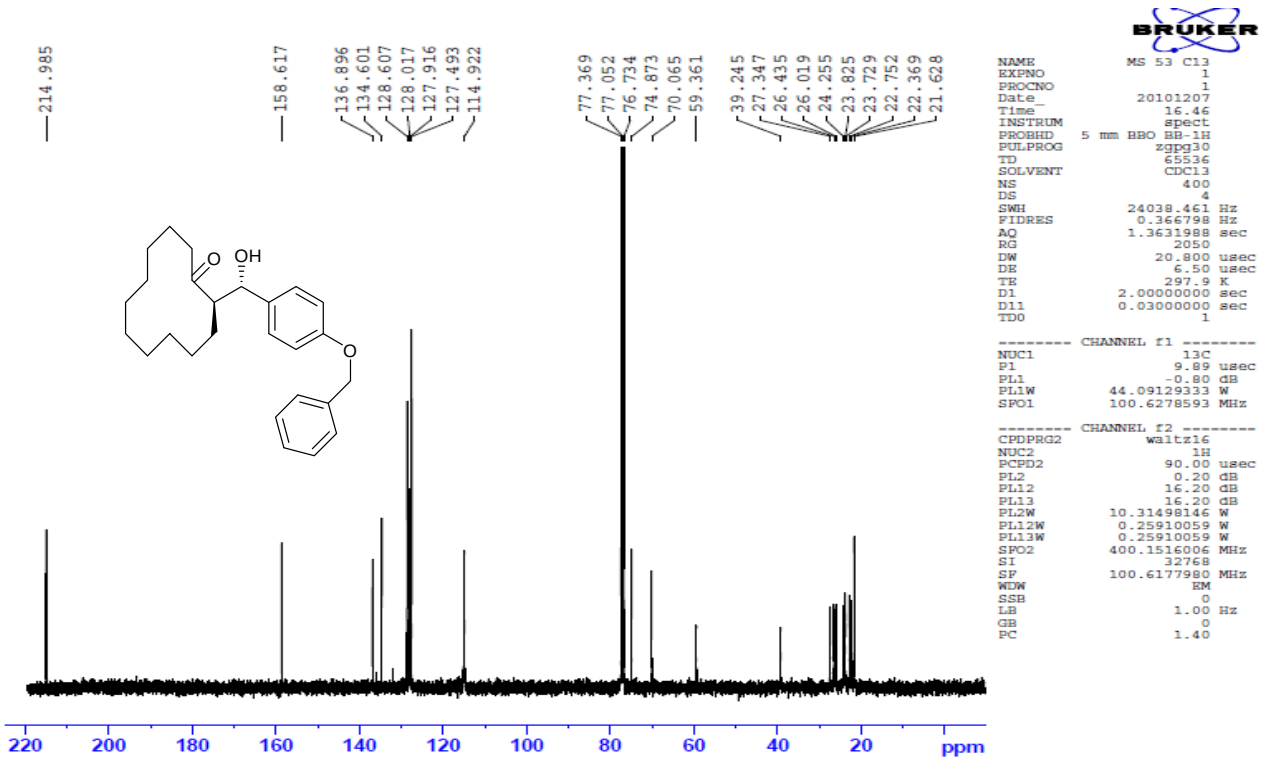
1	Peak1	5.117	Found	4356360	45.84	554288	49.49	Bv	4.356e+006	Q20	90
2	Peak2	5.420	Found	5147810	54.16	565786	50.51	vb	5.148e+006	Q20	133

^{1}H NMR of compound (4g)



C^{13} NMR of compound (4g)



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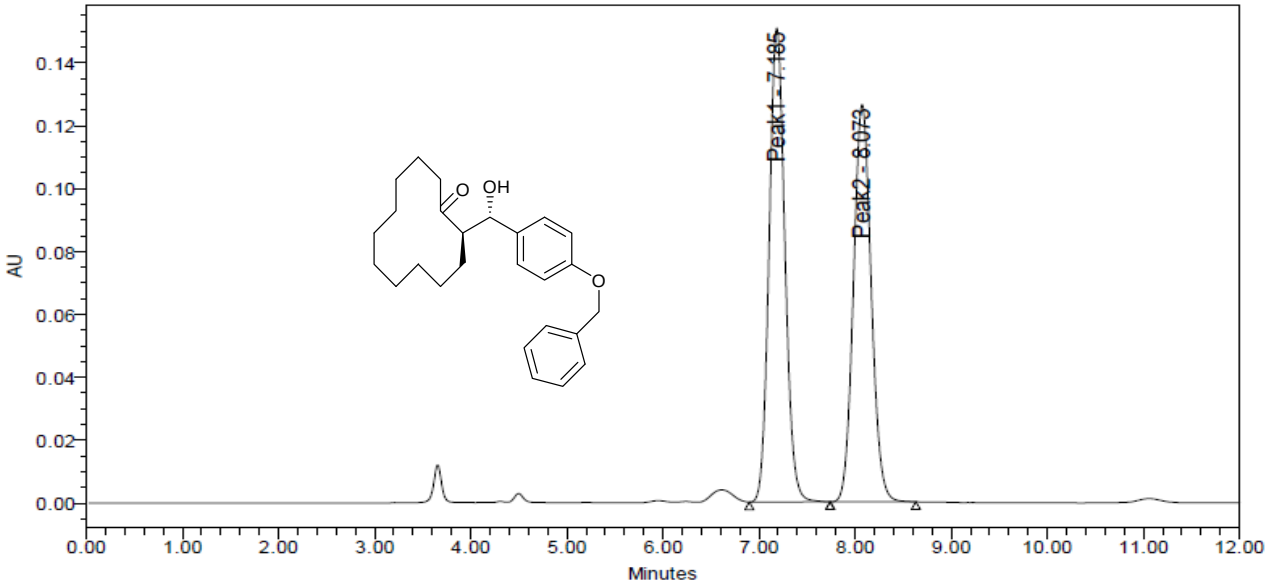
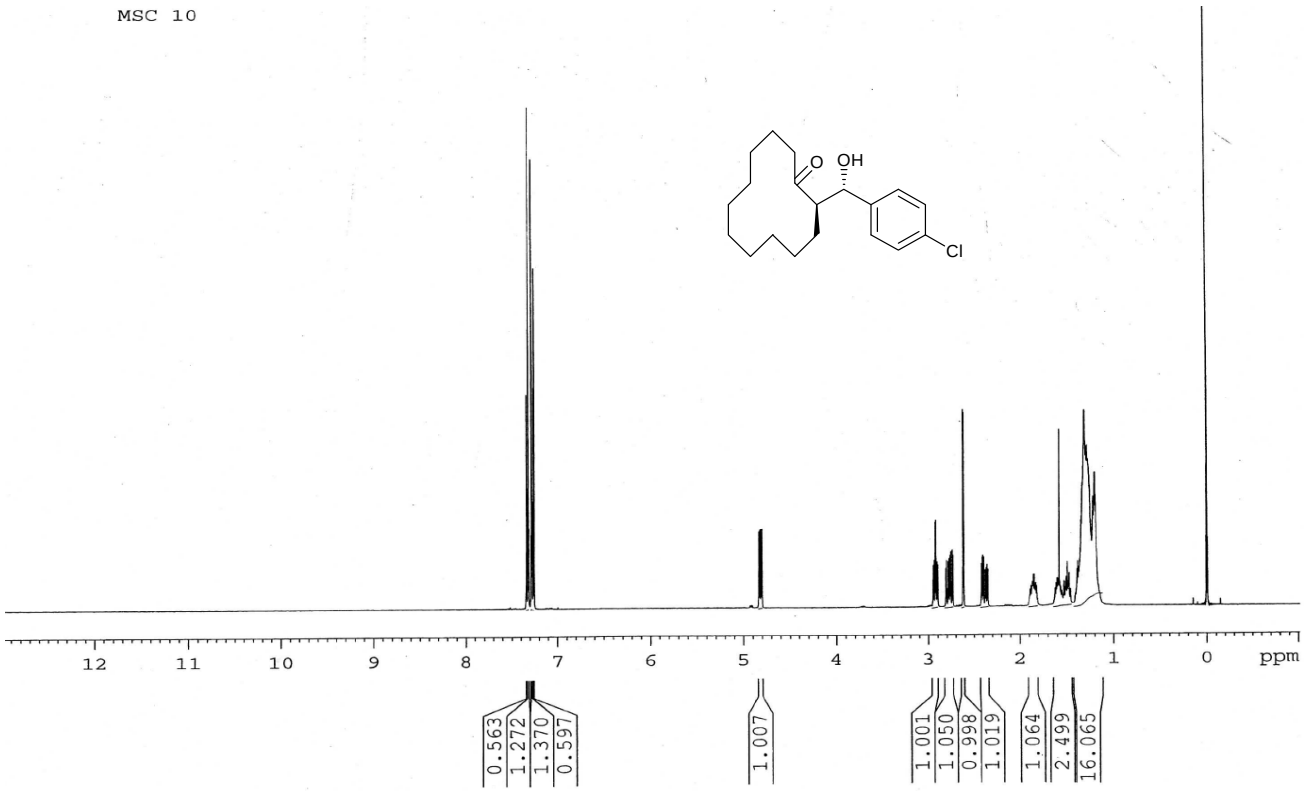


	Peak Name	RT (min)	Peak Type	Area (µV*sec)	% Area	Height (µV)	% Height	Integration Type	Response	Peak Codes	Points Across Peak
1	Peak1	7.185	Found	1719711	51.46	150602	54.40	BB	1.720e+006	Q20	252
2	Peak2	8.073	Found	1621956	48.54	126256	45.60	Bb	1.622e+006	Q20	268

^{1}H NMR of compound (4h)



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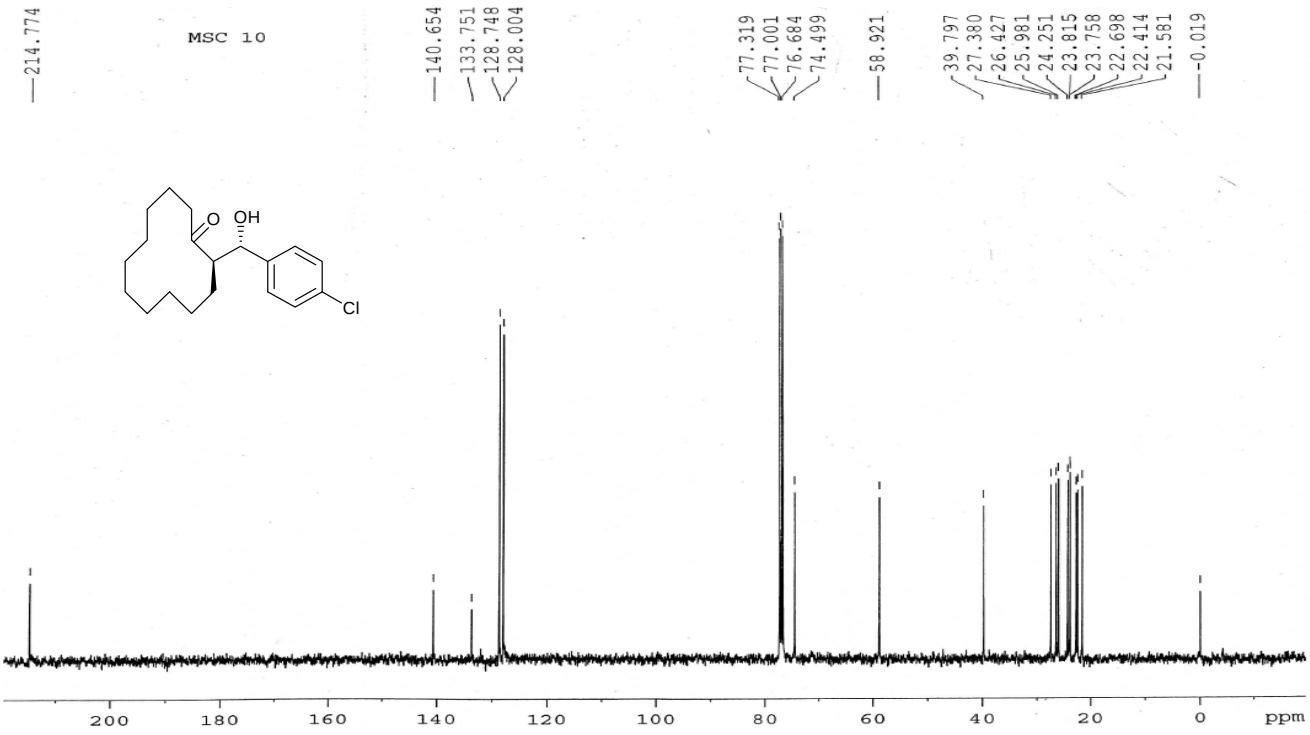

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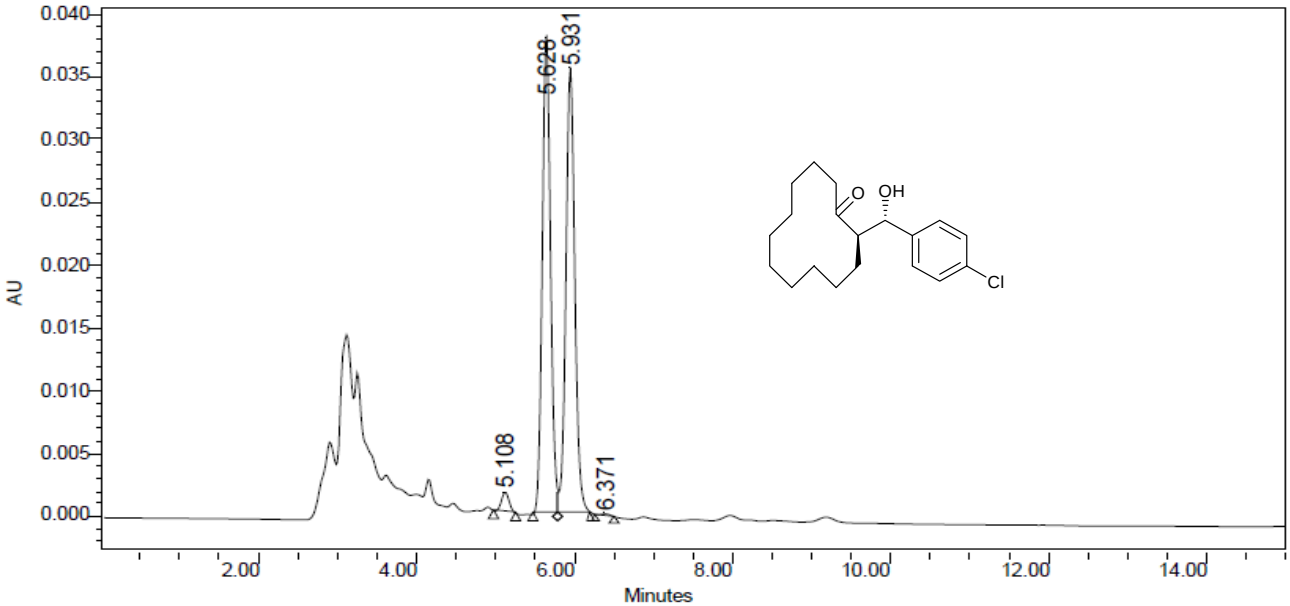
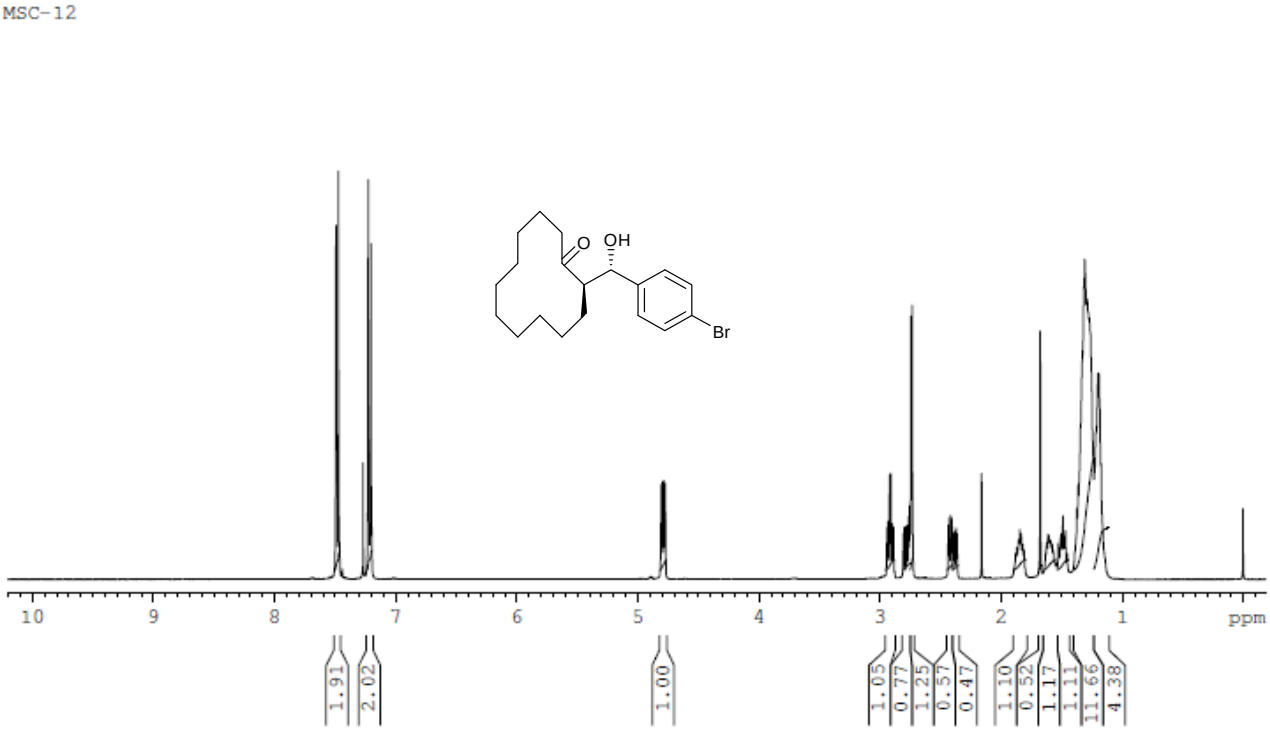


	RT (min)	Area (µV*sec)	% Area	Height (µV)	% Height
1	5.108	10858	1.91	1580	2.10
2	5.628	277330	48.89	38154	50.69
3	5.931	277841	48.98	35383	47.01
4	6.371	1195	0.21	153	0.20

^{1}H NMR of compound (4i)



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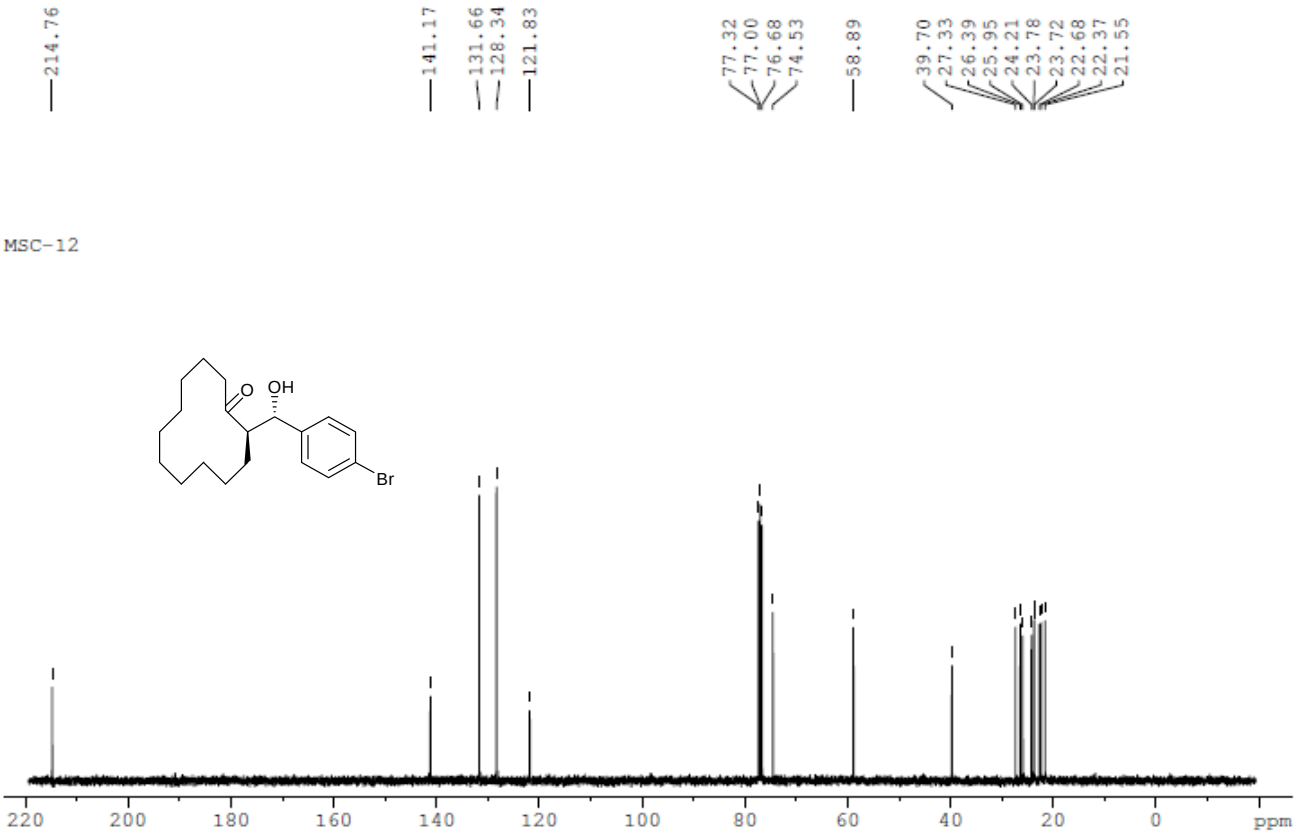

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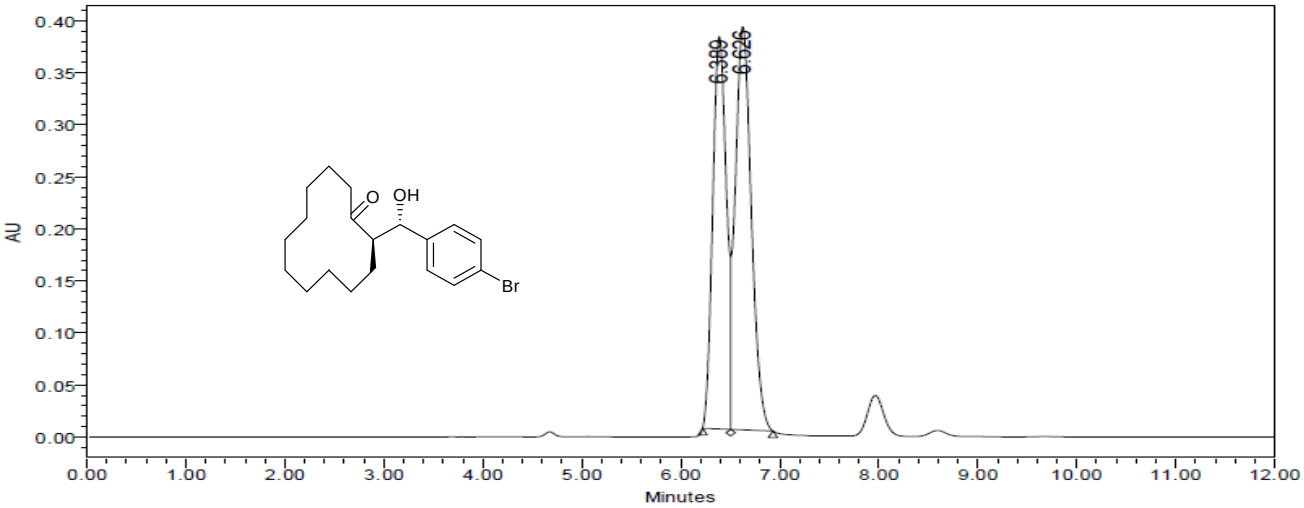

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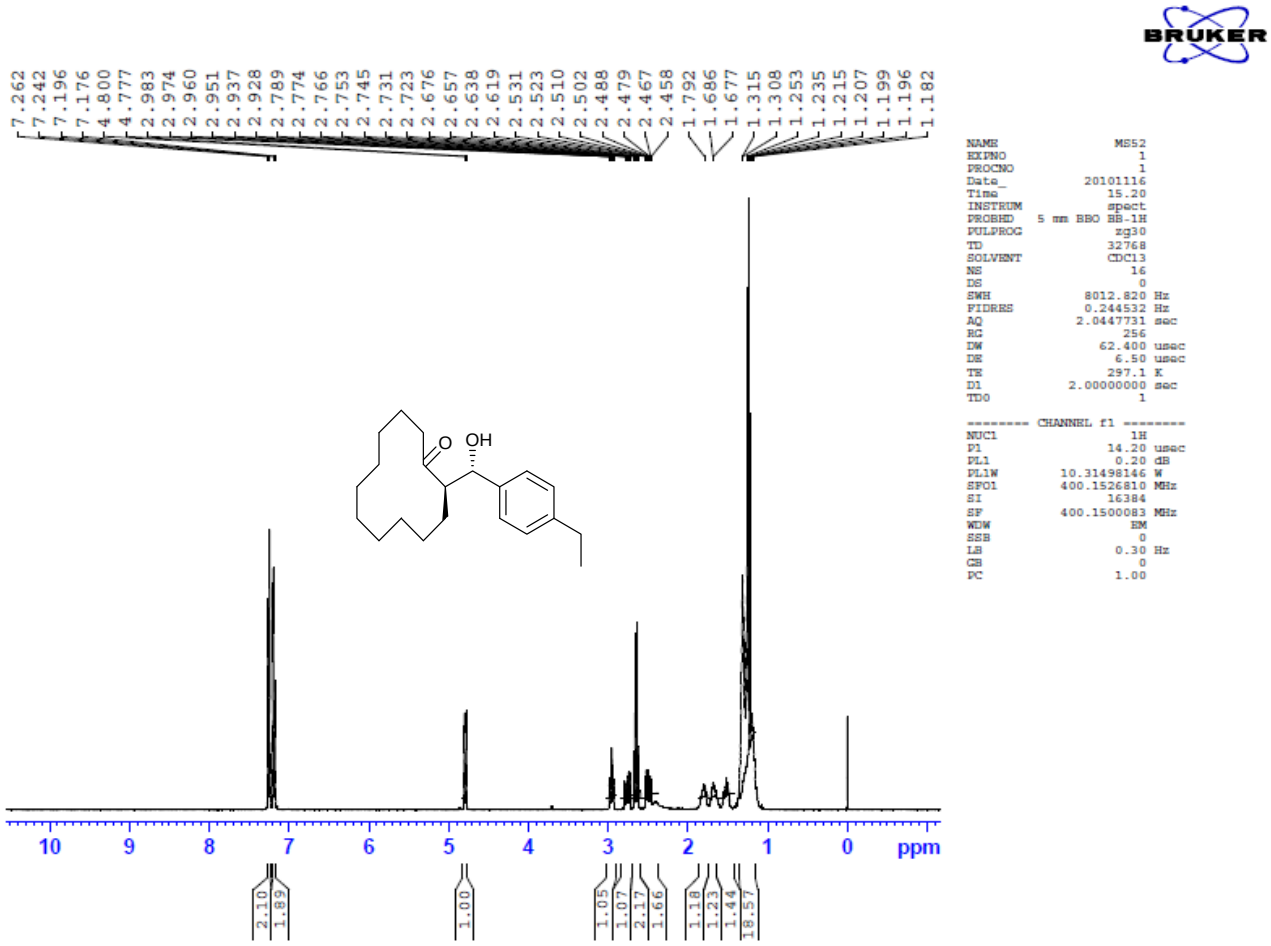
1	6.389	Unknown	3581622	44.84	377100	49.32	bv	85	6.220	6.503	6.220
2	6.626	Unknown	4405274	55.16	387503	50.68	vb	128	6.503	6.930	6.220

^{1}H NMR of compound (4j)



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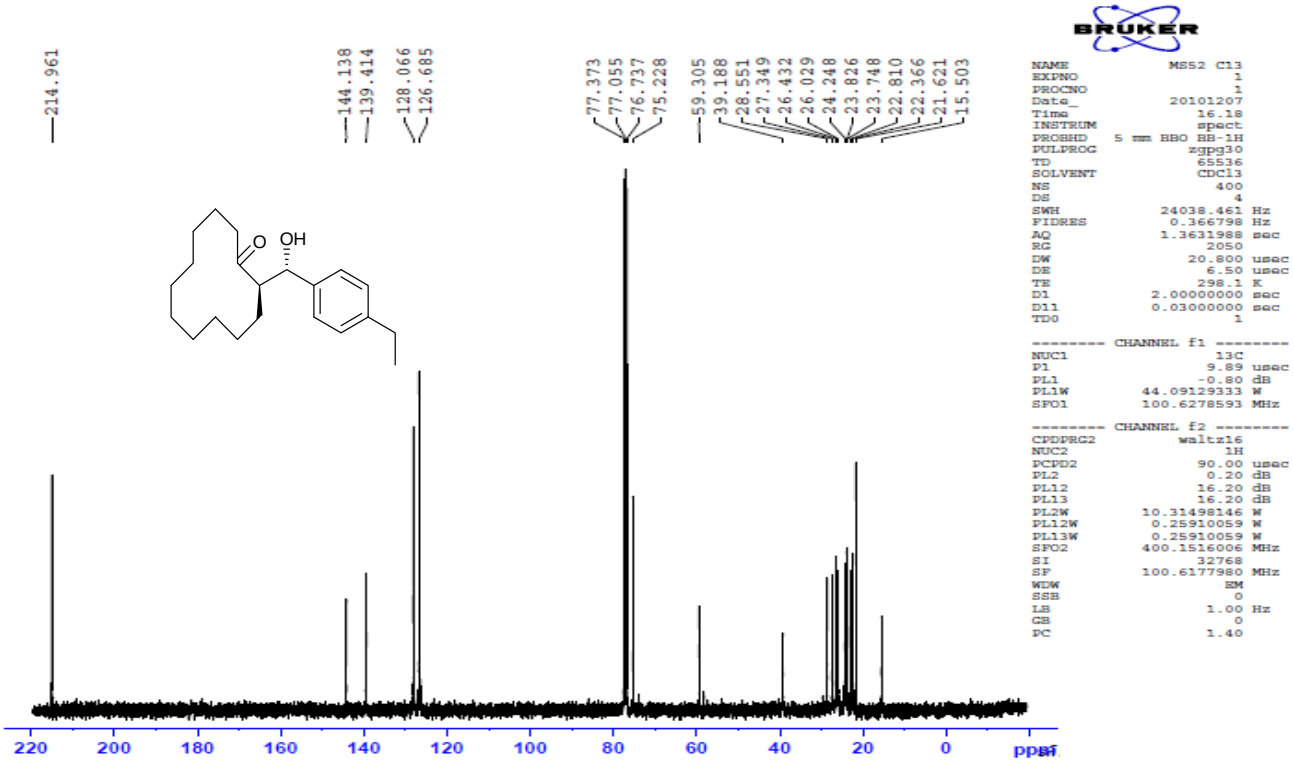

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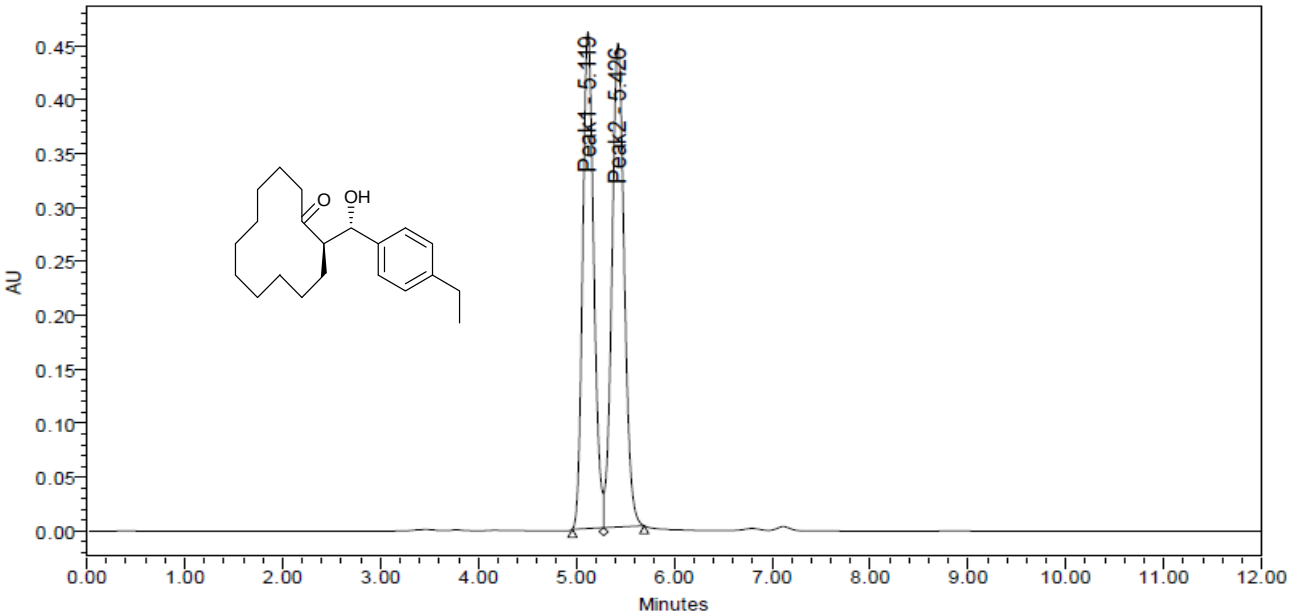

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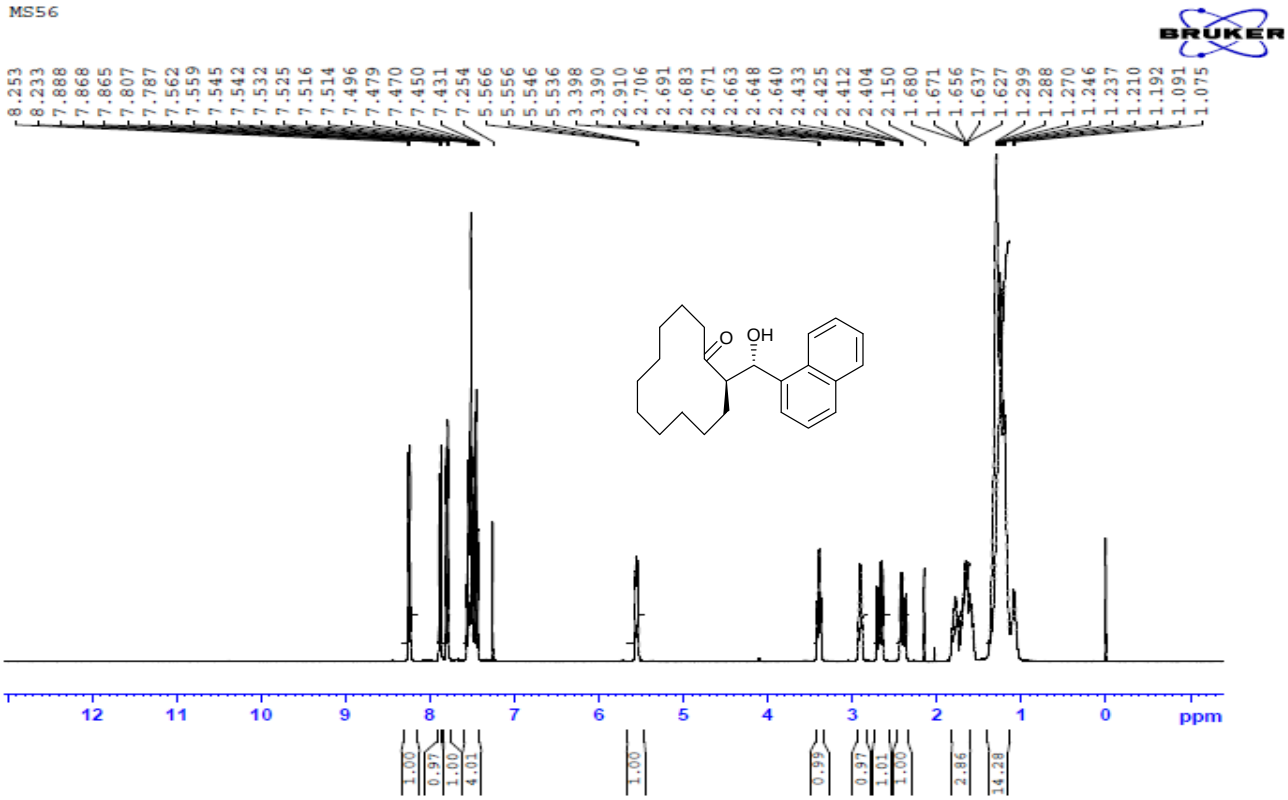
1	Peak1	5.119	Found	3626419	48.04	460458	50.65	Bv	3.626e+006	Q20	96
2	Peak2	5.426	Found	3922514	51.96	448698	49.35	vb	3.923e+006	Q20	124

^{1}H NMR of compound (4k)



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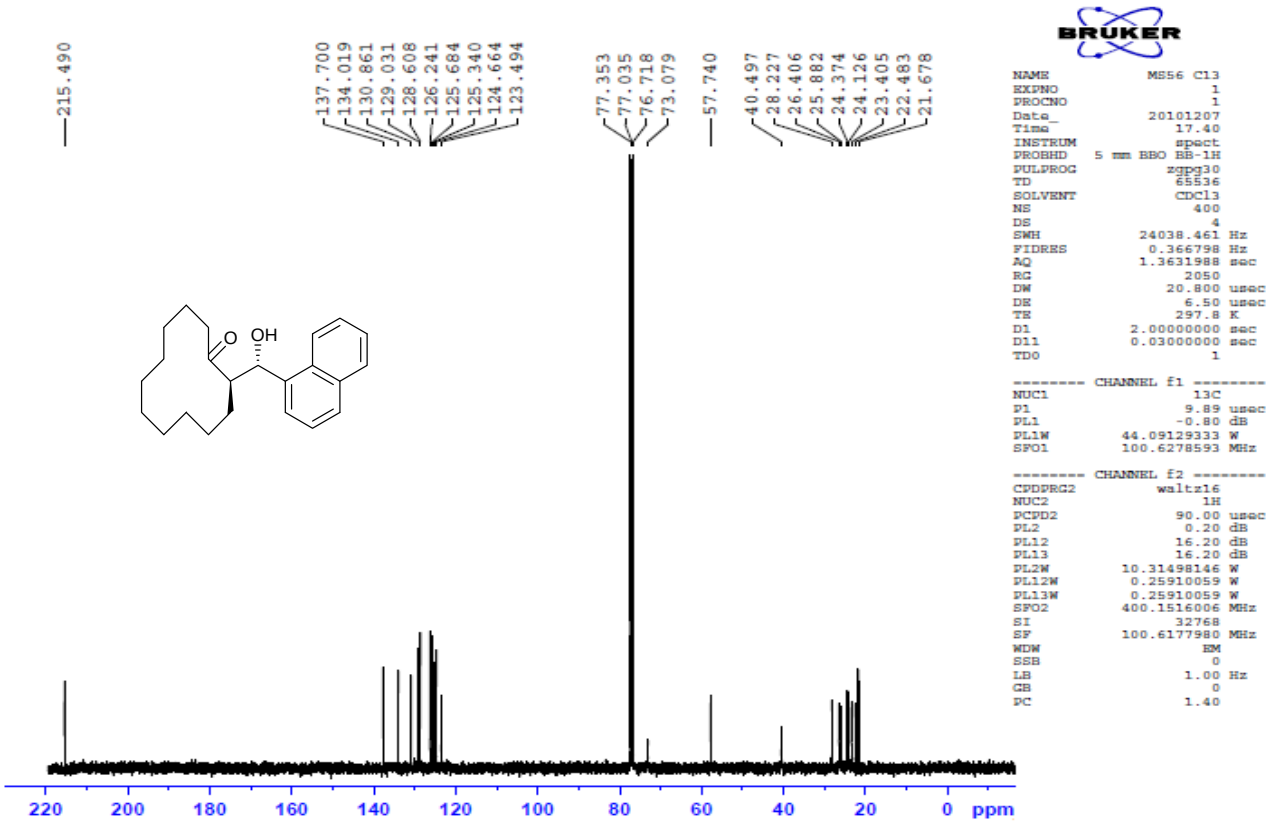

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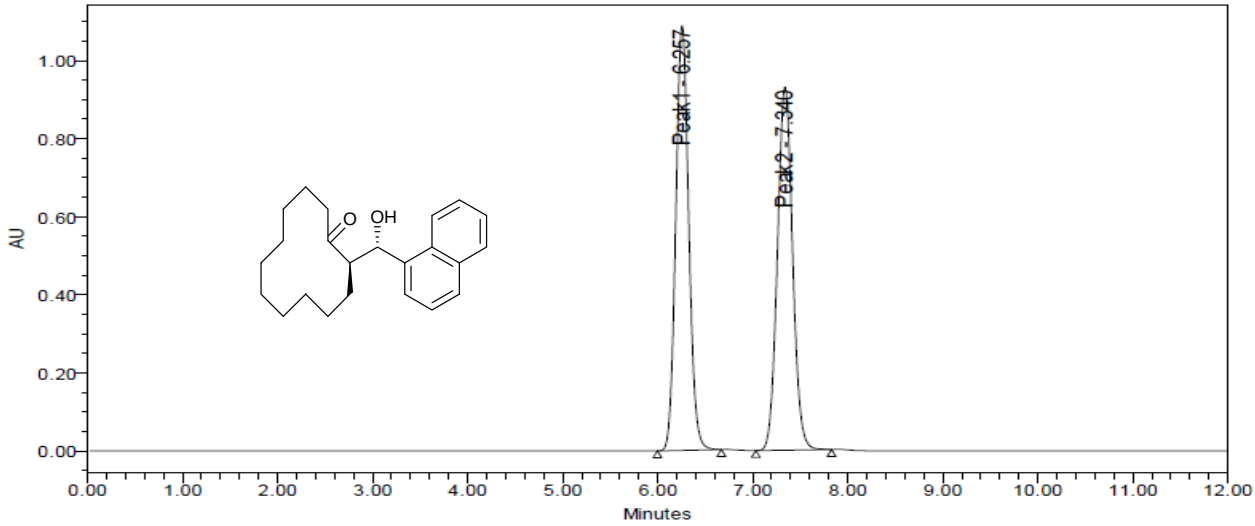

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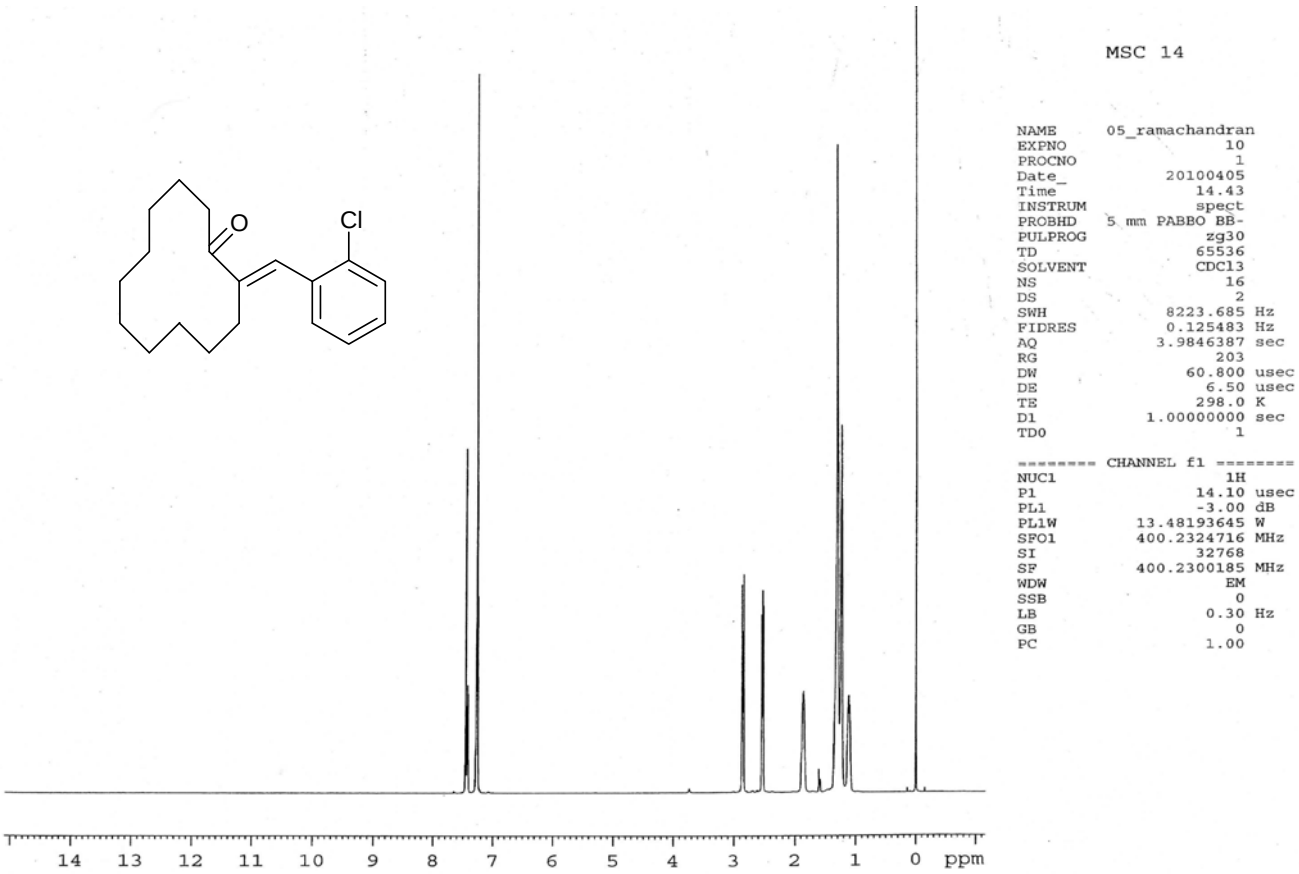
^{1}H NMR of compound (5a)

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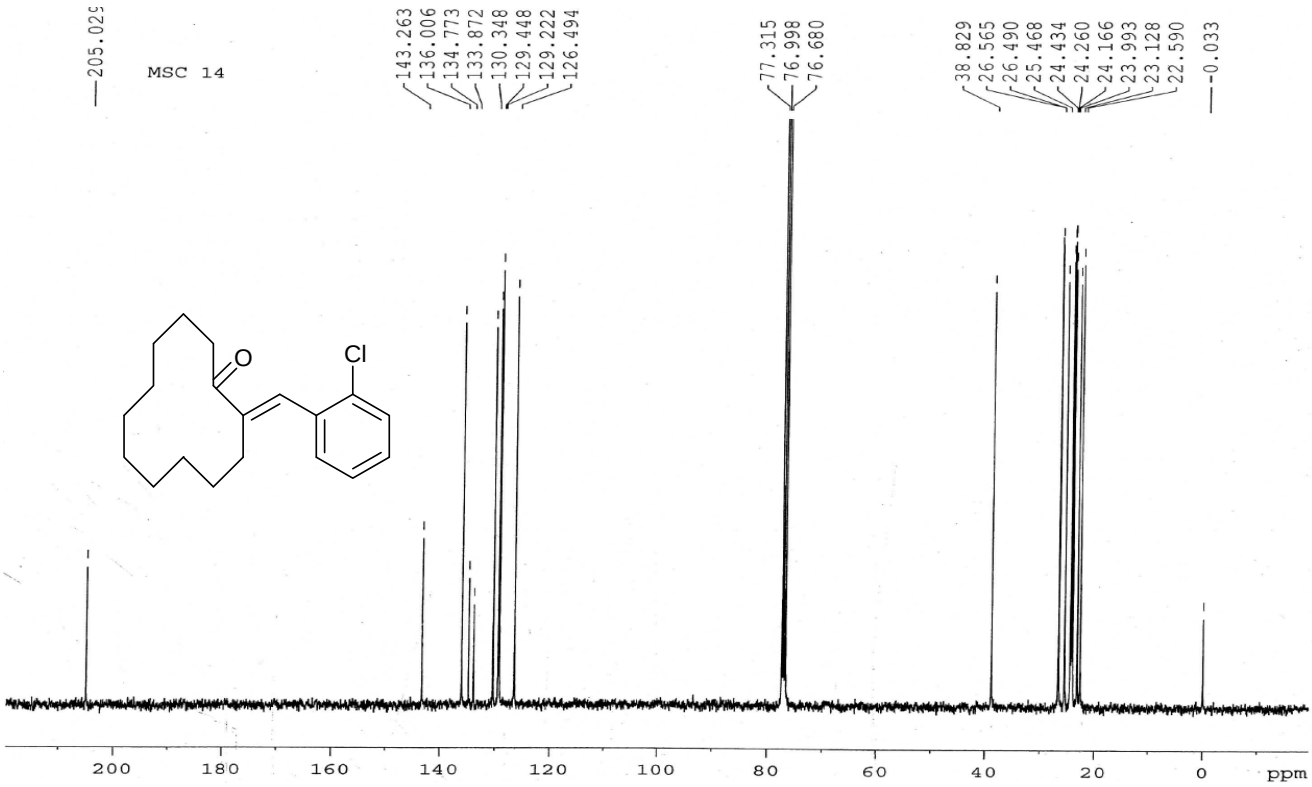
C^{13} NMR of compound (5a)



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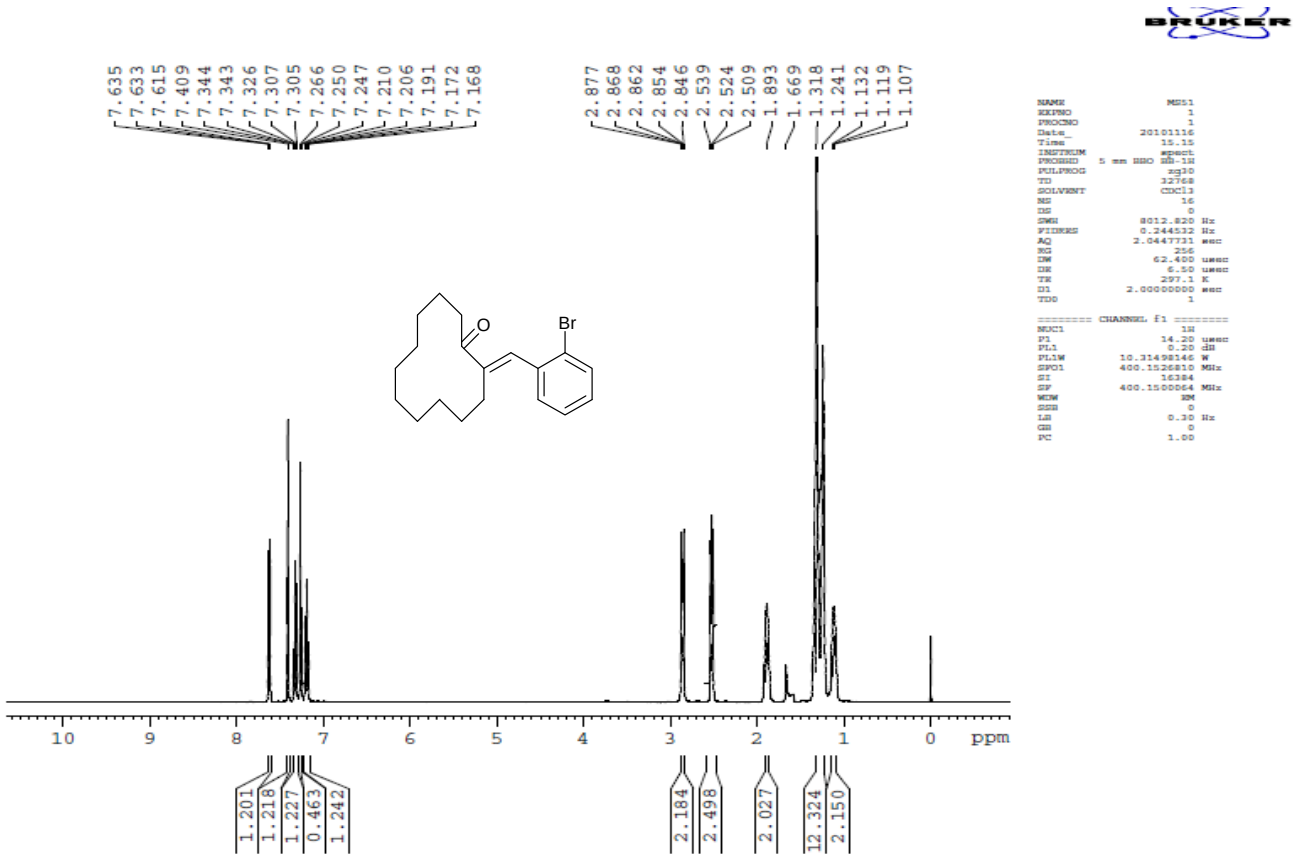

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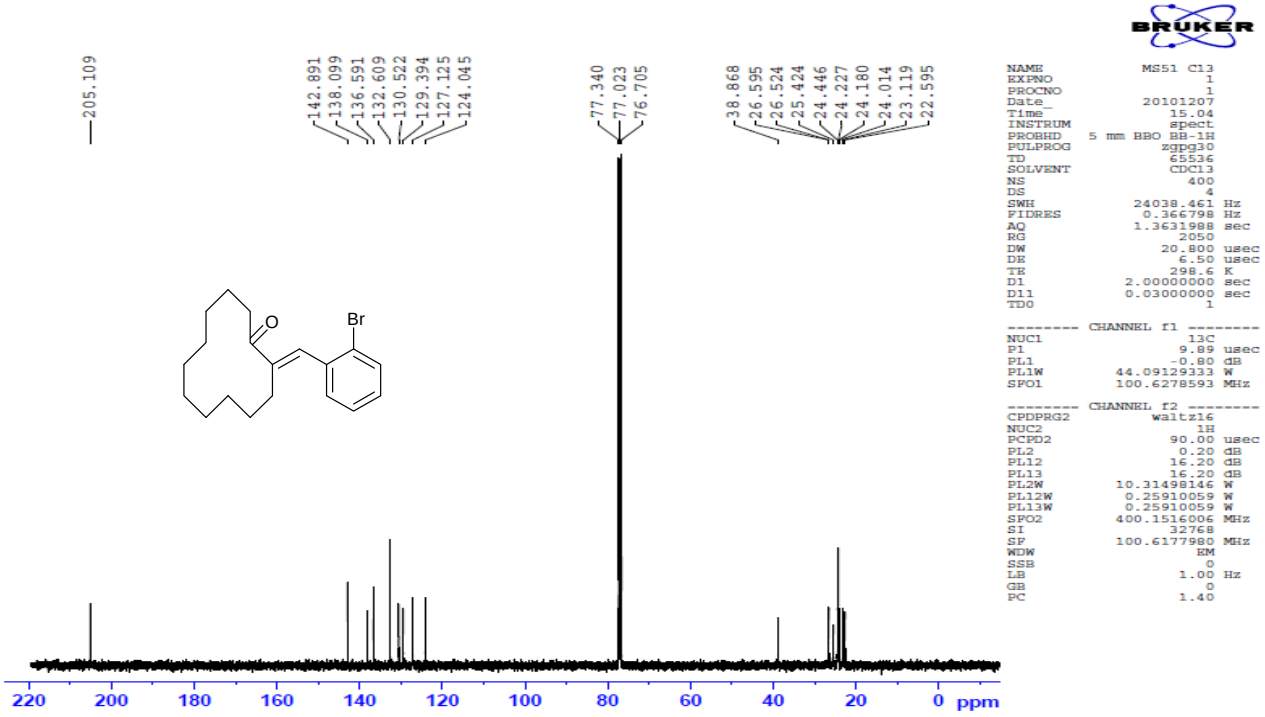

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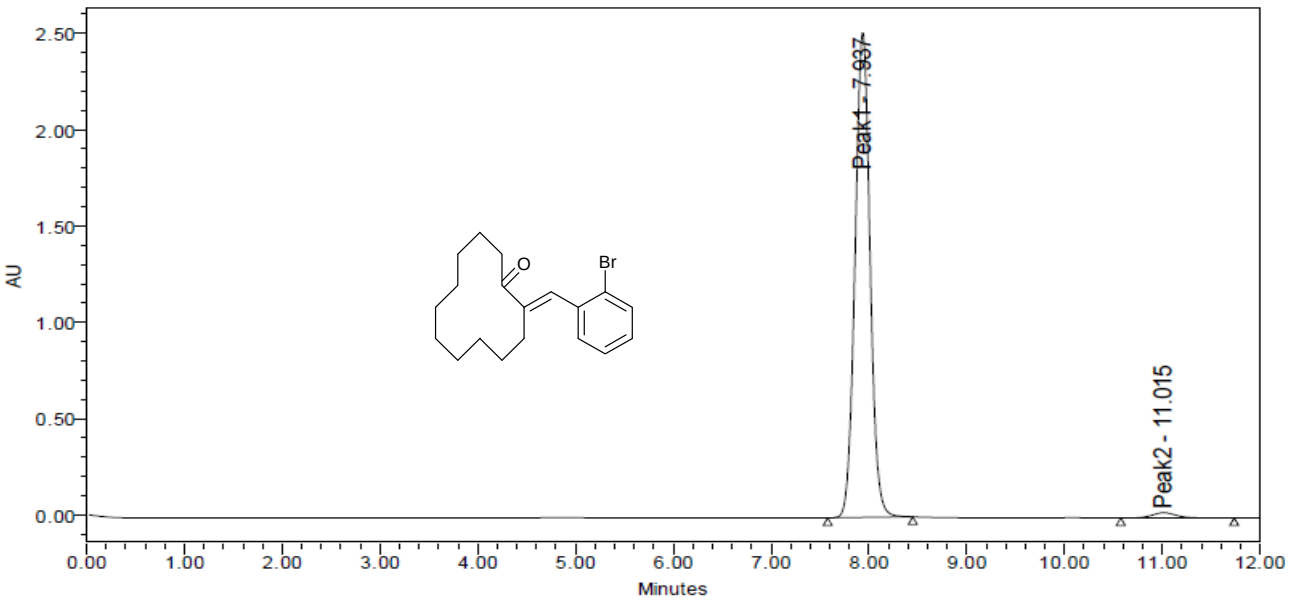

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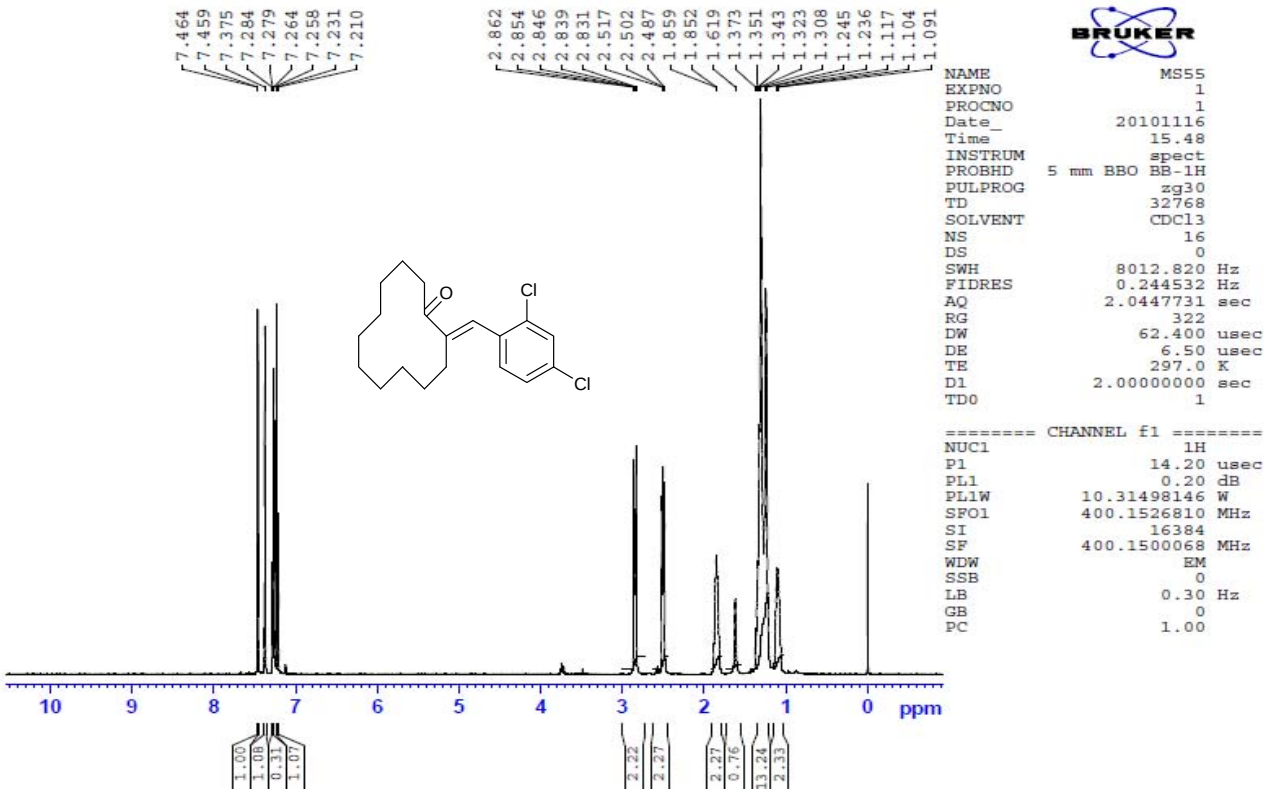
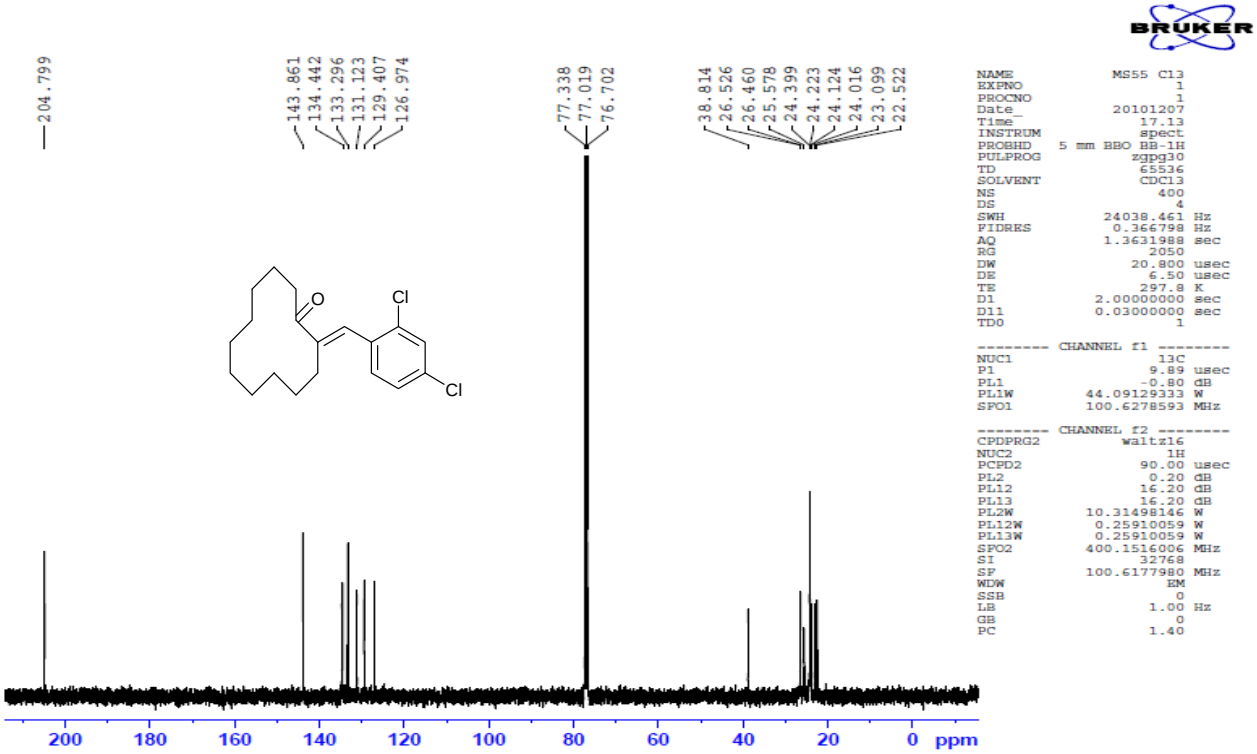
1	Peak1	7.937	Found	26835380	98.42	2515964	98.96	Bb	2.684e+007	Q20
2	Peak2	11.015	Found	431897	1.58	26517	1.04	BB	4.319e+005	Q20

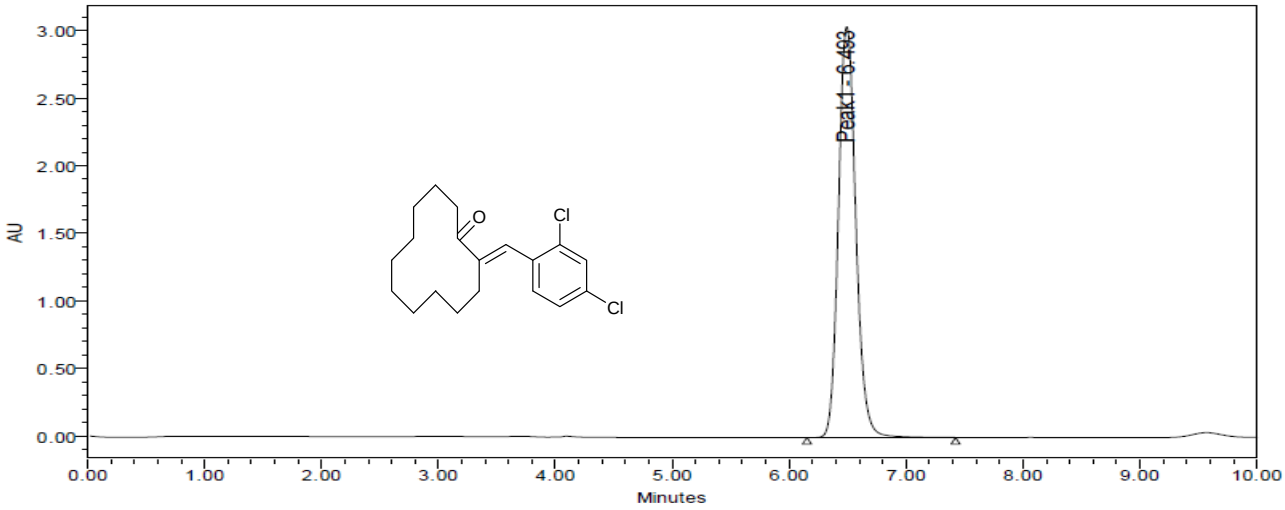
^{1}H NMR of Compound (5c)



C^{13} NMR of Compound (5c)



HPLC Data of compound (5c)



	Peak Name	RT (min)	Peak Type	Area (µV*sec)	% Area	Height (µV)	% Height	Integration Type	Response	Peak Codes
1	Peak1	6.493	Found	31411288	100.00	3039783	100.00	Bb	3.141e+007	Q20

Dynamic NMR spectra for Cyclododecanone at (25°C) in $CDCl_3$ solvent.

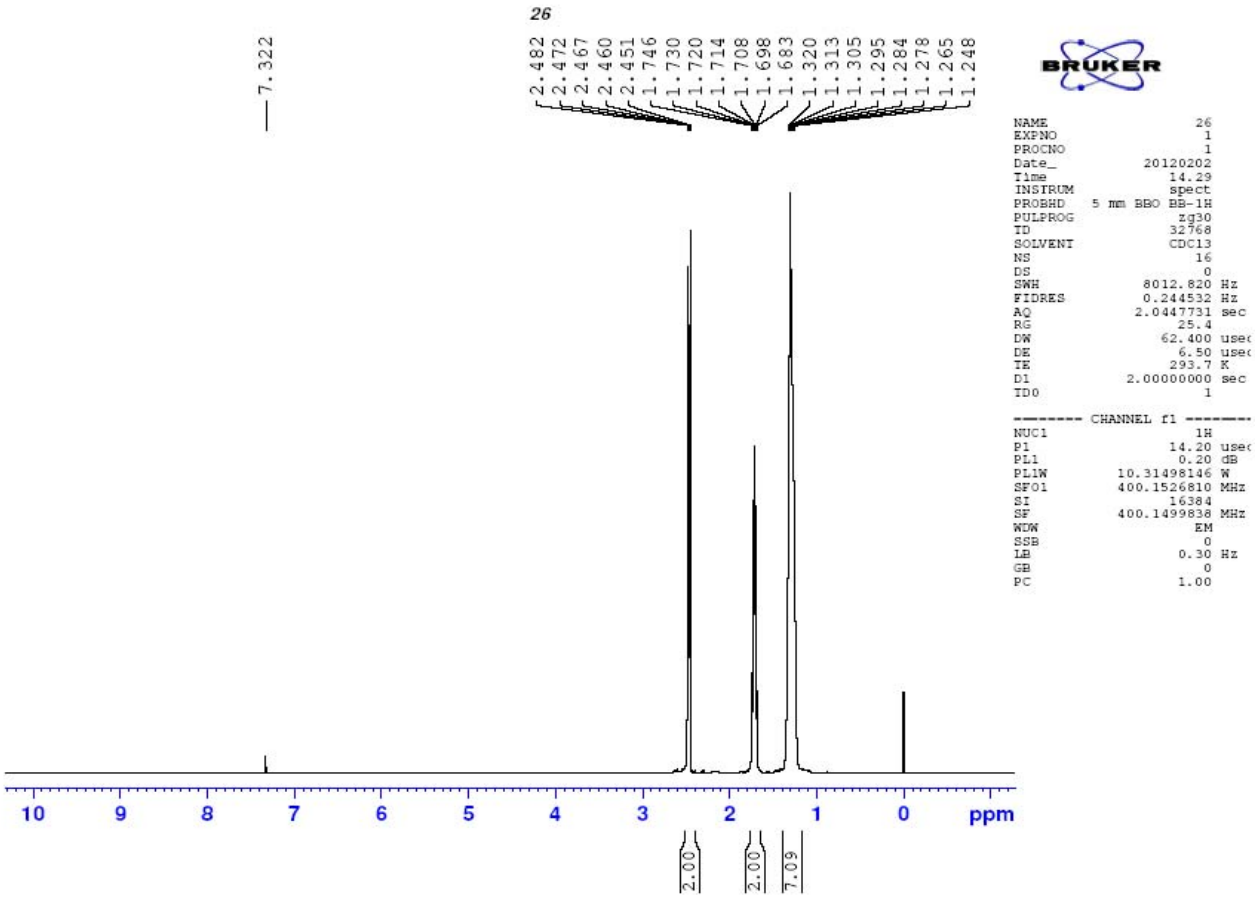


Table S1. Crystal data:

compounds	4f	4h	4i	4j	5c
Crystal Data					
Chemical formula	$C_{20}H_{30}O_2$	$C_{19}H_{27}ClO_2$	$C_{19}H_{27}BrO_2$	$C_{21}H_{32}O_2$	$C_{19}H_{24}Cl_2O$
Molecular Weight	302.44	322.86	367.32	316.47	339.28
Crystal size (mm)	0.6×0.4×0.2	0.4×0.4×0.4	0.4×0.4×0.3	0.4×0.3×0.2	0.4×0.4×0.3
Morphology	block, colorless	block, colorless	block, colorless	block, colorless	block, colorless
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	$P2_1$	$P2_1/n$	$P2_1/c$	$P2_1/c$	$P\bar{1}$
Unit cell parameters, a(Å), b(Å), c(c), □(°), □□(°), □□(°)	12.0425(6), 6.0319(3), 12.6615(6), 90, 106.214(5), 90	12.5731(3), 5.9925(1), 23.9975(5), 90, 104.709(2), 90	12.5505(8), 6.0048(5), 24.4004(15), 90, 104.889(7), 90	12.665(14), 5.8290(18), 25.713(9), 90, 100.94(5), 90	8.0433(6), 9.0769(10), 12.4273(10), 103.780(8), 92.678(6), 92.933(7)
Volume ($Å^3$)	883.14(7)	1748.82(6)	1777.2(2)	1864(2)	878.40(14)
Z/Z'	2/1	4/1	4/1	4/1	2/1
Cell measuring reflections	3020	15187	7291	1827	6274
□-range (°)	2.7-29.1	2.6-29.2	2.7-29.3	2.6-29.1	2.9-29.2
□(mm^{-1}) absorption correction	1.137, multi-scan	1.226, multi-scan	1.373, multi-scan	1.128, multi-scan	1.283, multi-scan
F(000)	332	696	768	696	360
D_x(calculated) (g cm^{-3})	0.071	0.224	2.318	0.070	0.369
Data Collection					
Radiation (Å)	0.71073 (MoKα)	0.71073 (MoKα)	0.71073 (MoKα)	0.71073 (MoKα)	0.71073 (MoKα)
Temperature (°K)	294	294	294	294	294
□ Range (°)	2.8-29.1	2.7-29.3	2.7-29.4	3.2-26.0	2.97-26.0

Indices	h = -15 → 16 k = -7 → 7 l = -17 → 15	h = -17 → 16 k = -8 → 8 l = -31 → 33	h = -16→ 16 k = -8 → 7 l = -32→32	h= -10→15 k= -4 → 7 l = -31→22	h= -9 → 9 k= -11 → 11 l= -15→ 15
Scan type	□ scans	□ scans	□ scans	□ scans	□ scans
Independent reflections	3638	4422	4476	3659	3443
Observed Reflections [I >2σ(I)]	2508	2967	2396	2320	2867
Refinement					
Final Indices	R = 0.0432, wR = 0.0846	R = 0.0430, wR = 0.1124	R = 0.0320, wR = 0.0655	R = 0.0676, wR = 0.1733	R = 0.0359, wR = 0.0889
Goodness of fit (S)	0.942	1.067	0.850	1.039	1.010
Extinction coefficient	nil	nil	nil	nil	0.026(3)
$(\Delta/\sigma)_{max}$	0.0	0.0	0.0	0.0	0.0
$\Delta\rho_{max}$ and $\Delta\rho_{min}$ (e $Å^{-3}$)	0.122, -0.142	0.348, -0.239	0.351, -0.612	0.260, -0.238	0.207, -0.247
Data/restraints/ parameter	3638/204/1	4422/203/0	4476/203/0	3659/213/0	3443/200/0

$w = 1/[\square^2(F_0^2) + (aP)^2 + bP]$ where $P = (F_o^2 + 2F_c^2)/3$, parameters a and b are: 0.0473, 0.0 (**4f**), 0.0619, 0.1253 (**4h**), 0.0378, 0.0 (**4i**), 0.0984, 0.1388 (**4j**) and 0.0436, 0.2428 (**5c**), respectively.