

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042123\
 Data File : BM039552.D
 Acq On : 21 Apr 2023 14:54
 Operator : CG/JU
 Sample : 02270-23
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-15-5-7-20230412

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039552.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.913	315	319	327	rVB	81195	117110	1.98%	0.362%
2	5.384	393	399	417	rBV	1793626	2769318	46.82%	8.568%
3	6.996	667	673	701	rBV	1607723	2957822	50.01%	9.151%
4	7.819	806	813	833	rBV	562607	990047	16.74%	3.063%
5	8.990	1005	1012	1030	rBV	958014	1788486	30.24%	5.533%
6	10.625	1283	1290	1303	rBV	708067	1319601	22.31%	4.083%
7	13.095	1703	1710	1738	rBV	2775850	4272999	72.25%	13.220%
8	14.478	1938	1945	1962	rBV	1081778	1726495	29.19%	5.341%
9	15.842	2172	2177	2187	rBV	42960	84194	1.42%	0.260%
10	15.972	2192	2199	2220	rBV	1885346	2952764	49.93%	9.135%
11	17.224	2406	2412	2427	rBV	1217383	1974513	33.39%	6.109%
12	18.124	2560	2565	2581	rBV	191286	426793	7.22%	1.320%
13	19.295	2760	2764	2772	rVB2	36354	61656	1.04%	0.191%
14	19.407	2779	2783	2794	rBV2	77999	164662	2.78%	0.509%
15	19.860	2854	2860	2875	rBV	4663156	5914274	100.00%	18.297%
16	21.136	3072	3077	3086	rBV3	216799	468886	7.93%	1.451%
17	21.418	3120	3125	3139	rBV	1454186	2208490	37.34%	6.833%
18	23.783	3521	3527	3542	rVB2	1041064	2124981	35.93%	6.574%

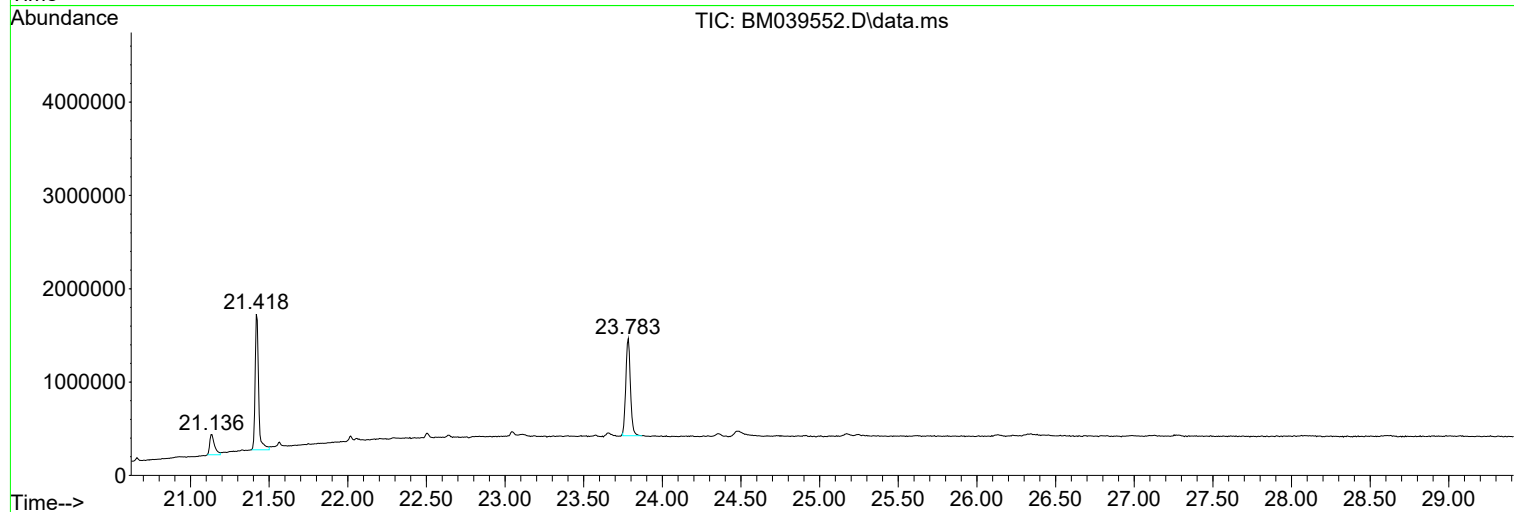
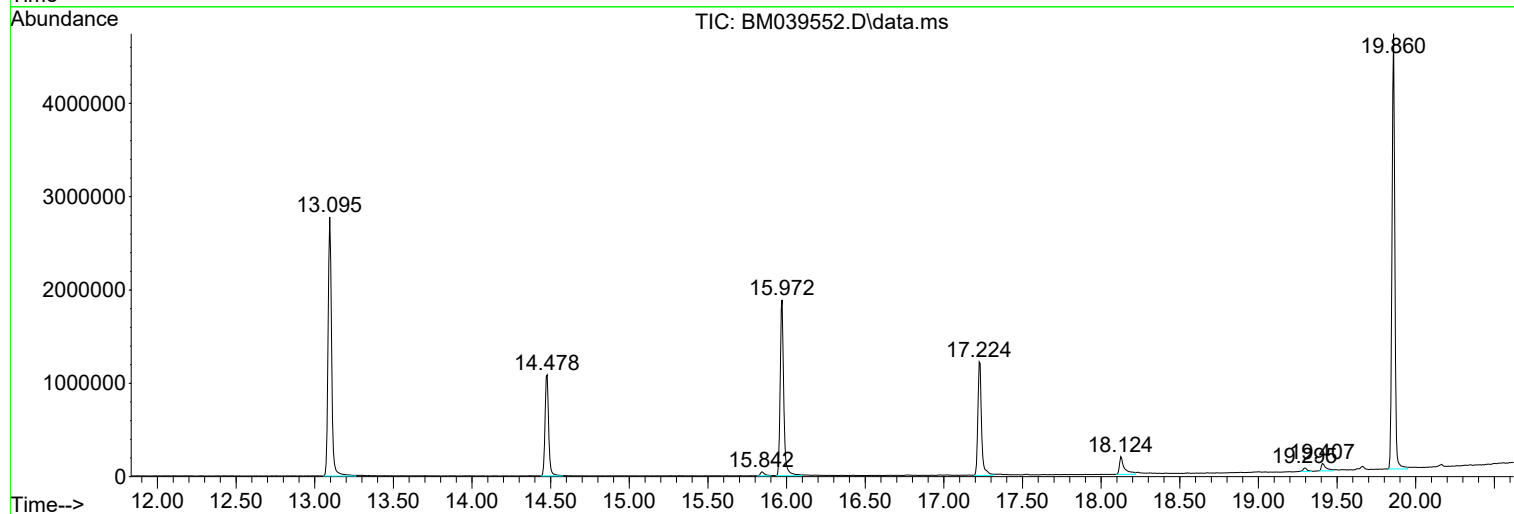
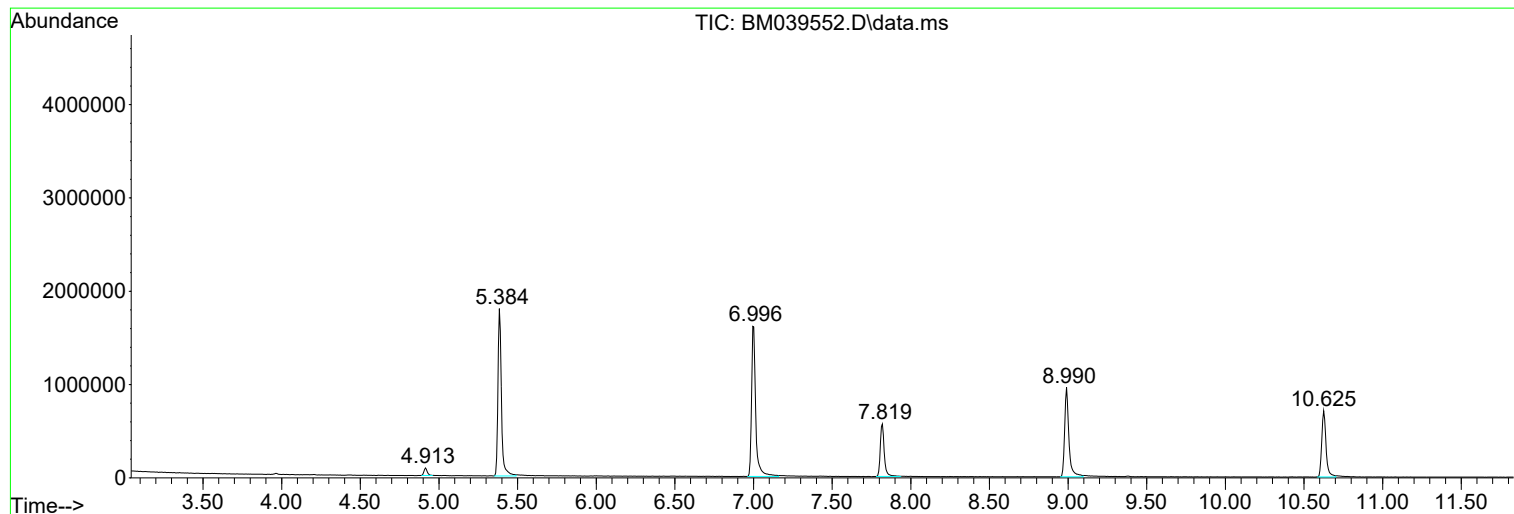
Sum of corrected areas: 32323091

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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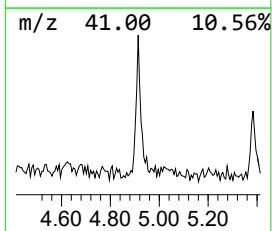
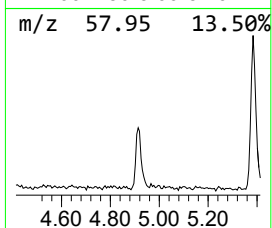
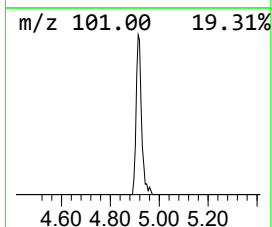
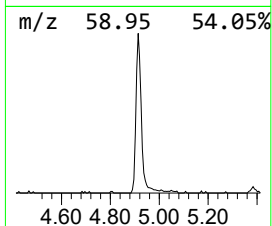
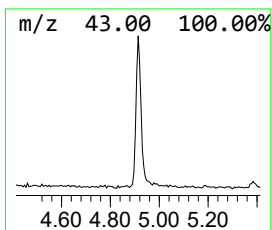
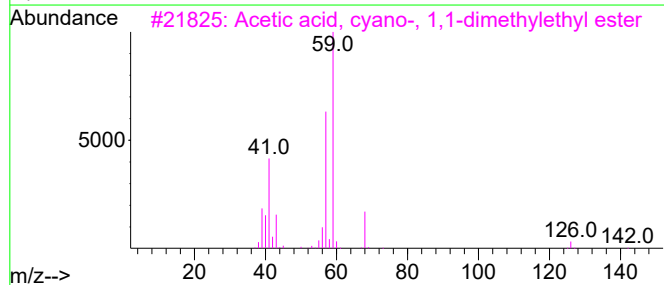
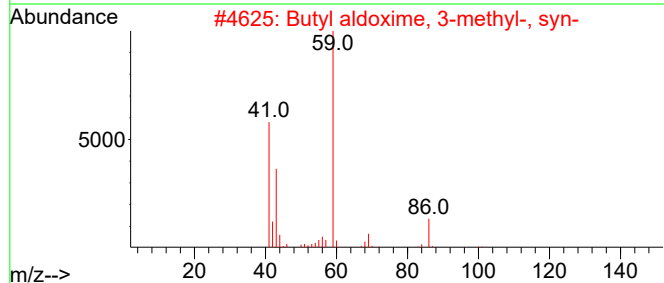
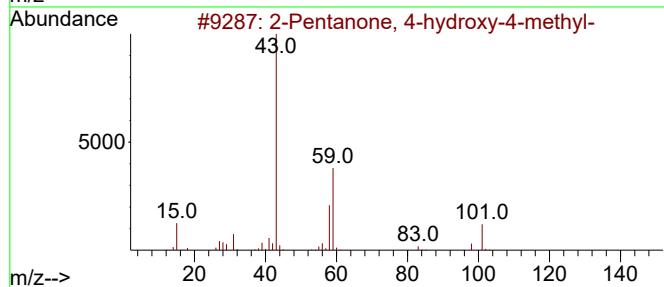
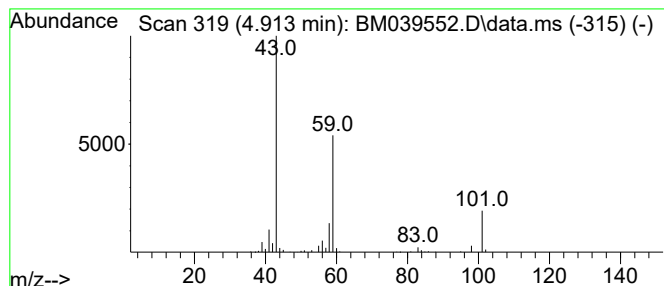
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.913	2.37 ng	117110	1,4-Dichlorobenzene-d4	7.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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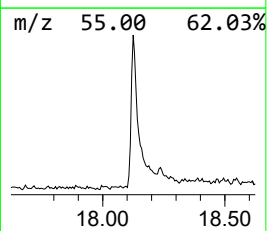
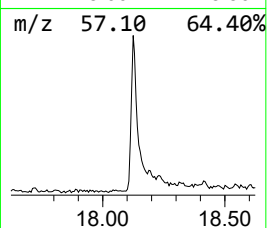
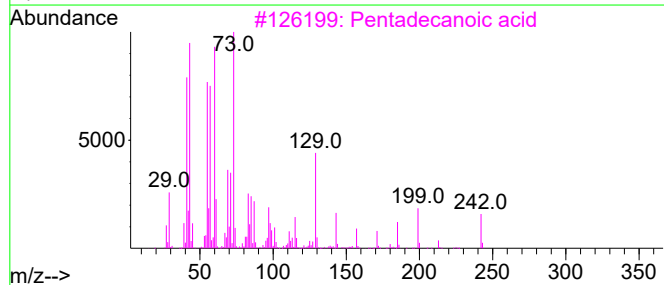
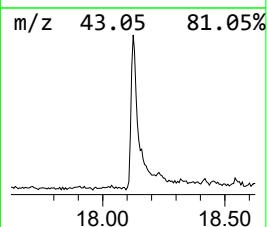
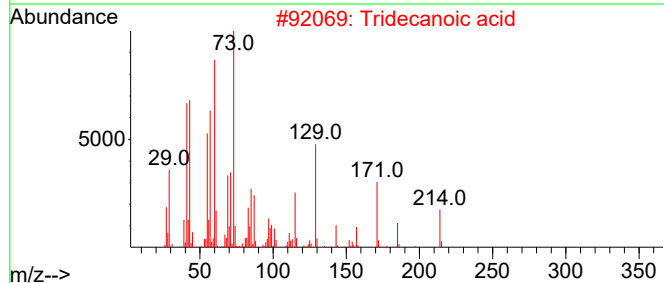
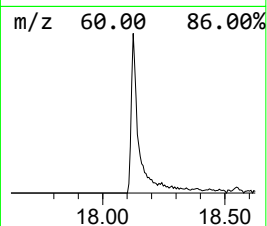
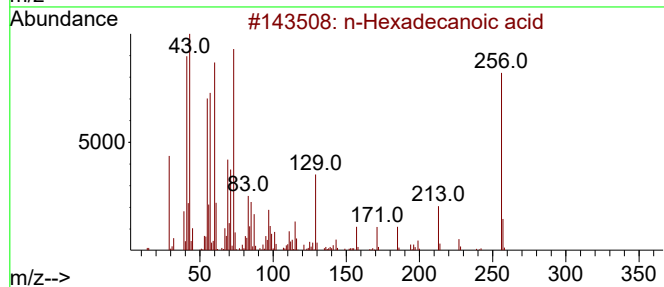
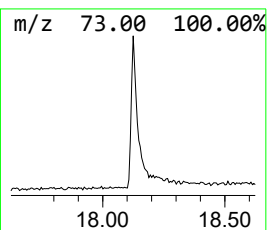
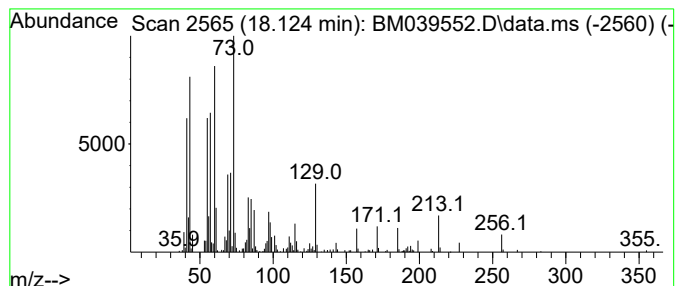
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.124	4.32 ng	426793	Phenanthrene-d10	17.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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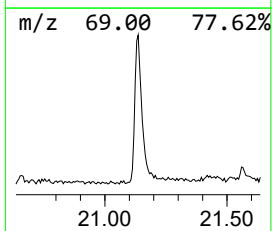
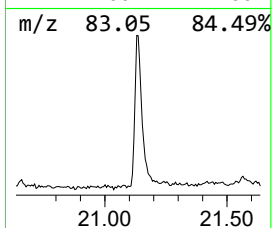
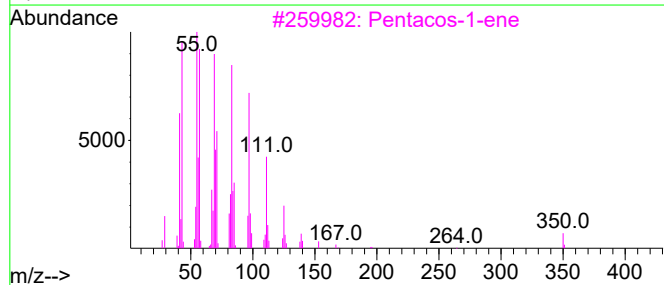
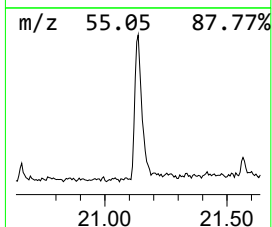
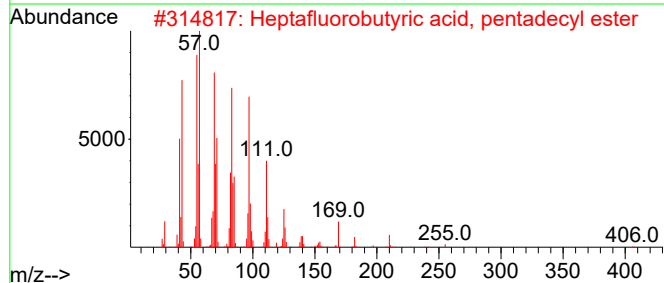
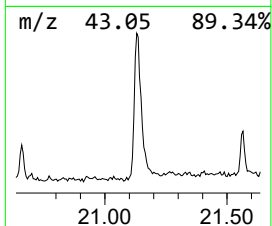
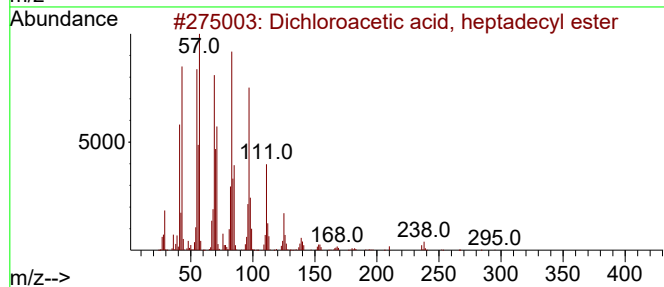
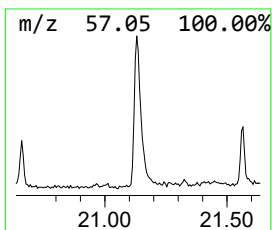
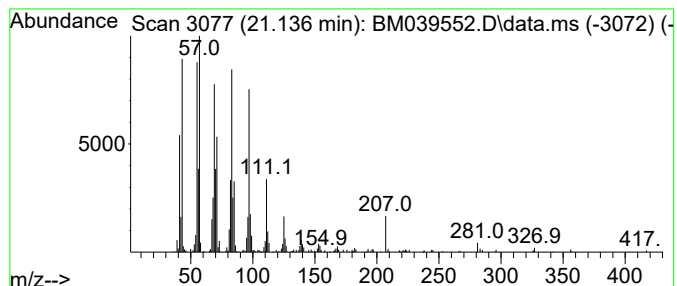
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Peak Number 3 Dichloroacetic acid, heptad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.136	4.25 ng	468886	Chrysene-d12	21.418

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.913	2.4	ng	117110	1	7.819	990047	20.0
n-Hexadecanoic ...	18.124	4.3	ng	426793	4	17.224	1974510	20.0
Dichloroacetic ...	21.136	4.3	ng	468886	5	21.418	2208490	20.0