

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080822\
 Data File : BM036158.D
 Acq On : 08 Aug 2022 23:40
 Operator : CG/JU
 Sample : N3961-14
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RVE-180

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-BM080122.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036158.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.946	310	316	321	rBV	210565	287696	2.93%	0.483%
2	5.434	392	399	408	rBV	4052073	5824826	59.37%	9.787%
3	7.051	667	674	691	rBV	3758385	5840475	59.53%	9.814%
4	7.845	801	809	816	rBV	972587	1530666	15.60%	2.572%
5	9.016	1000	1008	1023	rBV	2340962	3790289	38.63%	6.369%
6	10.645	1276	1285	1292	rBV	1240465	2079443	21.19%	3.494%
7	13.116	1697	1705	1717	rBV	5515865	8019676	81.74%	13.475%
8	14.210	1885	1891	1898	rVB2	60952	103737	1.06%	0.174%
9	14.486	1931	1938	1944	rBV	1766299	2502389	25.51%	4.205%
10	15.974	2185	2191	2198	rBV	4157033	5847554	59.60%	9.826%
11	17.227	2396	2404	2408	rBV	2051796	2780304	28.34%	4.672%
12	17.268	2408	2411	2416	rVB	217957	282931	2.88%	0.475%
13	17.362	2423	2427	2431	rVB	75409	103879	1.06%	0.175%
14	18.127	2550	2557	2566	rBV2	378615	695423	7.09%	1.169%
15	18.292	2581	2585	2590	rBV3	62753	111793	1.14%	0.188%
16	19.021	2705	2709	2712	rBV2	69219	114251	1.16%	0.192%
17	19.286	2749	2754	2760	rBV	438309	583411	5.95%	0.980%
18	19.645	2811	2815	2825	rVB	513557	802927	8.18%	1.349%
19	19.851	2845	2850	2860	rVB	7948350	9811034	100.00%	16.485%
20	21.121	3060	3066	3072	rBV3	811681	1388263	14.15%	2.333%
21	21.403	3109	3114	3118	rBV	2459050	3393262	34.59%	5.702%
22	23.039	3389	3392	3398	rBV2	432931	669587	6.82%	1.125%
23	23.762	3509	3515	3522	rVB2	1550810	2950156	30.07%	4.957%

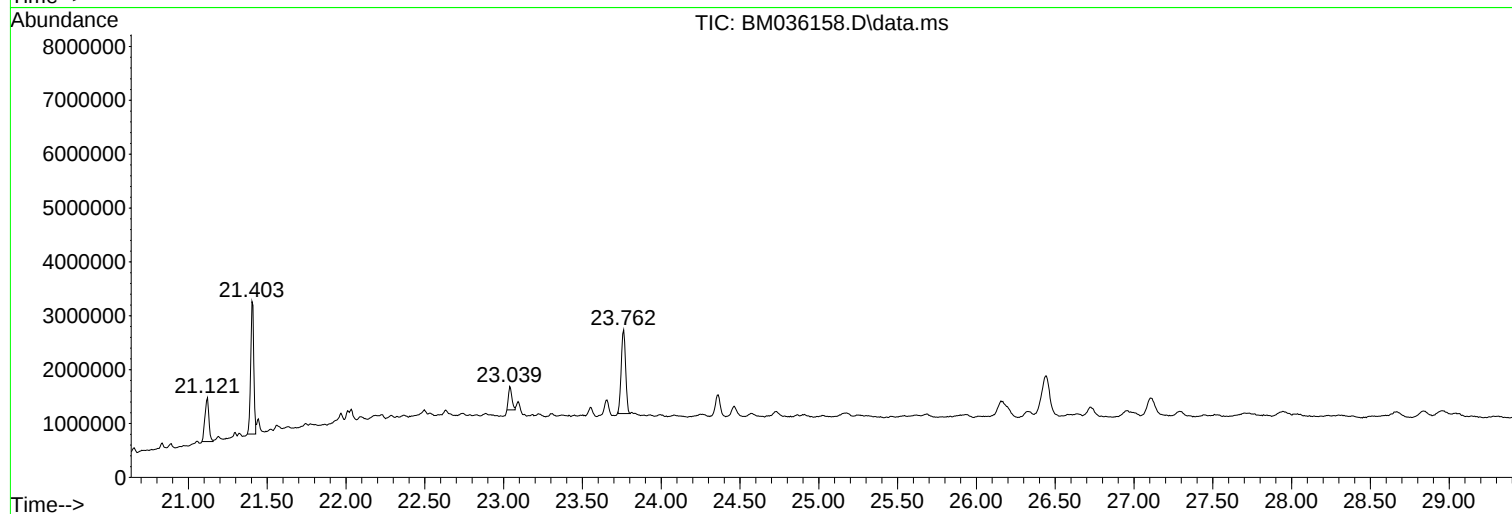
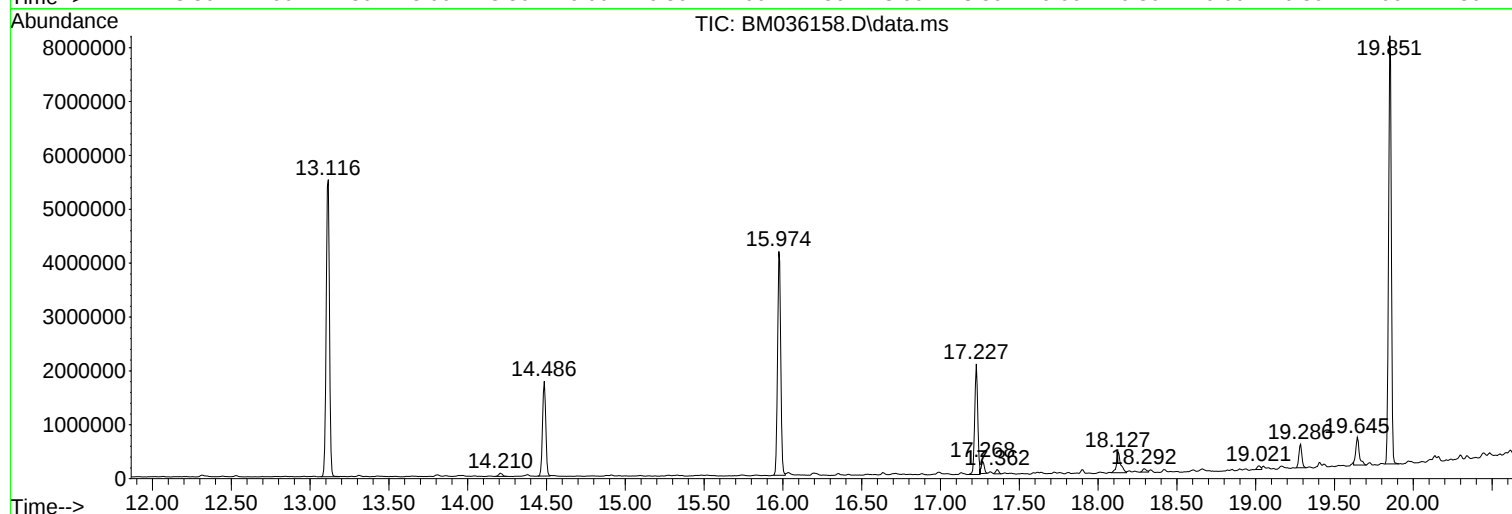
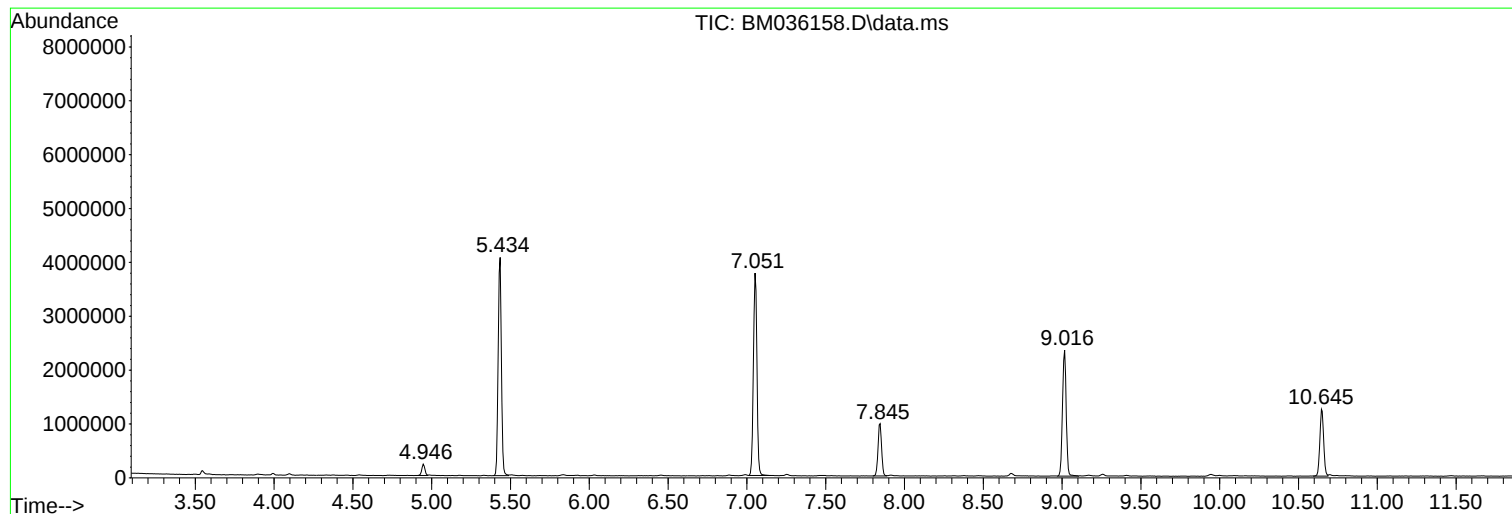
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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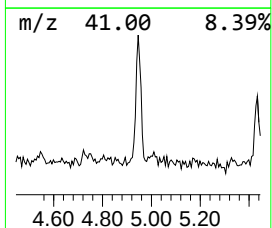
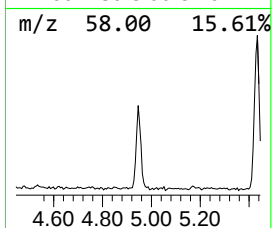
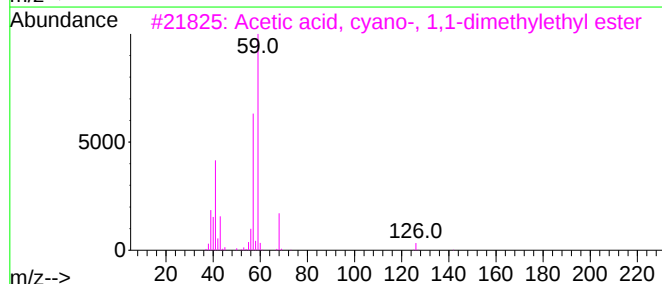
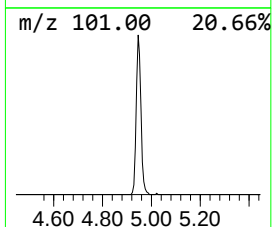
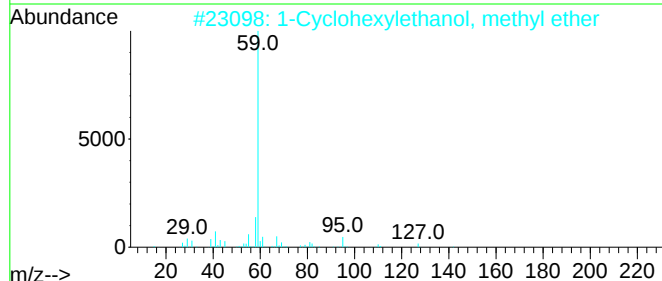
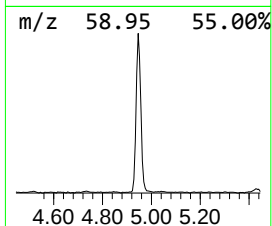
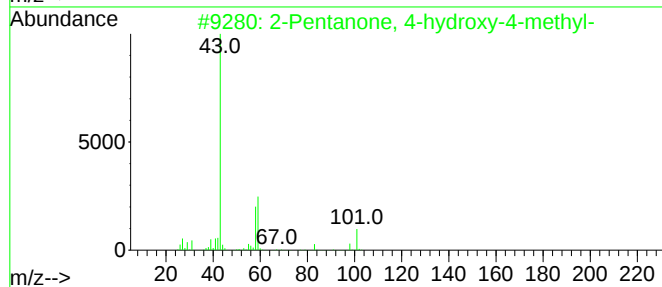
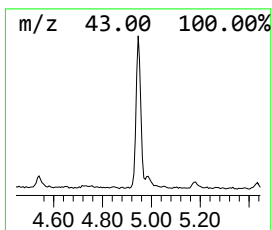
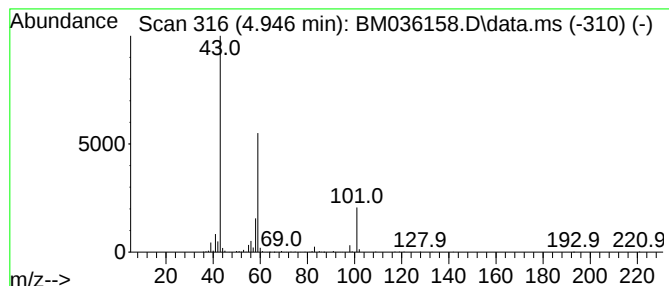
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.946	3.76 ng	287696	1,4-Dichlorobenzene-d4	7.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	1-Cyclohexylethanol, methyl ether	142	C9H18O	1000365-12-8	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	17		
5	Acetone	58	C3H6O	000067-64-1	9		



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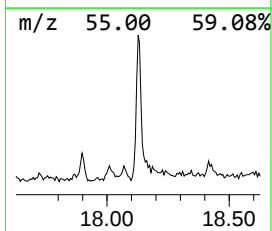
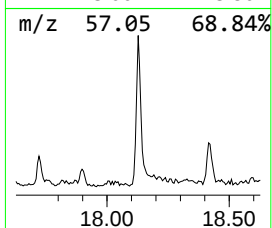
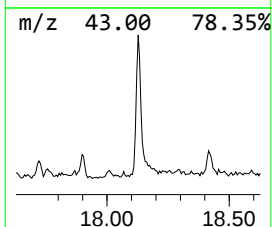
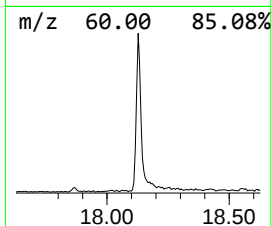
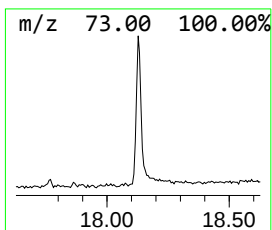
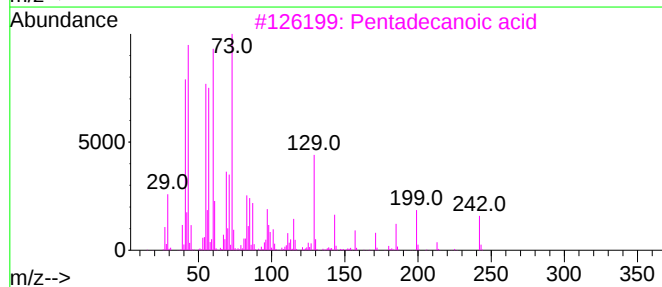
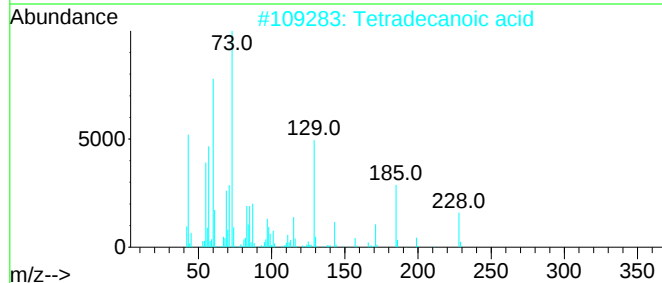
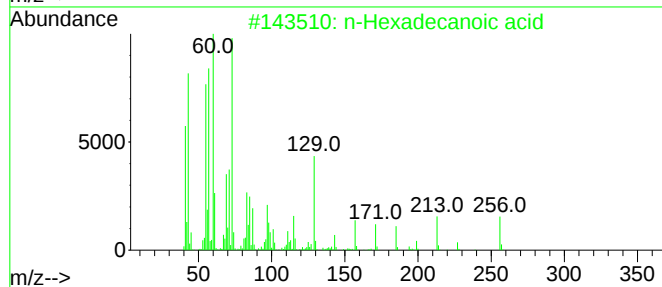
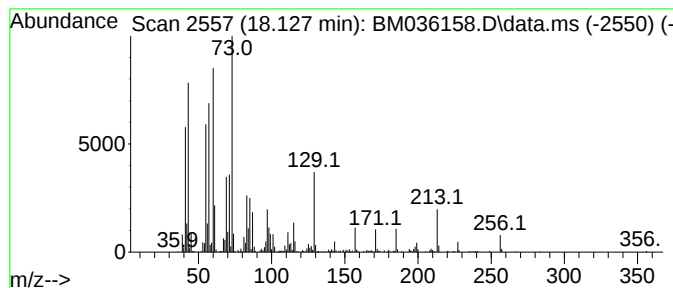
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	5.00 ng	695423	Phenanthrene-d10	17.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Octadecanoic acid	284	C18H36O2	000057-11-4	74



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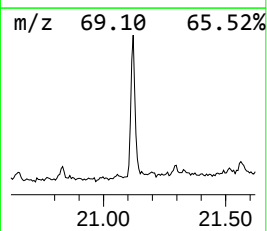
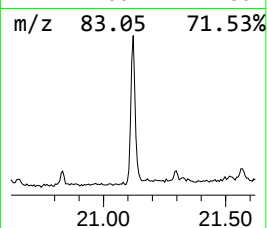
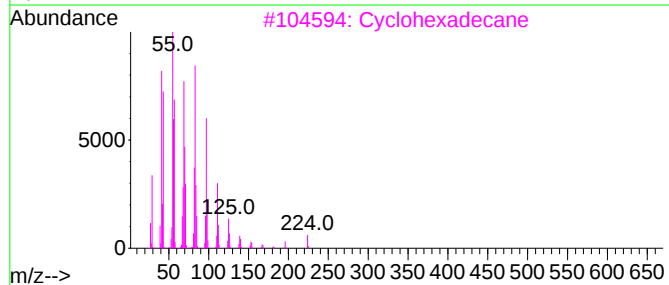
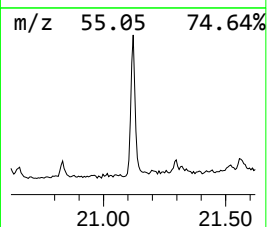
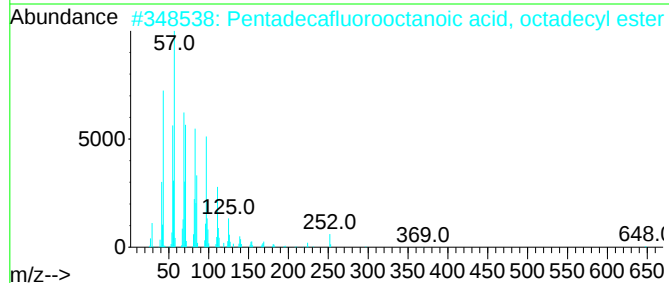
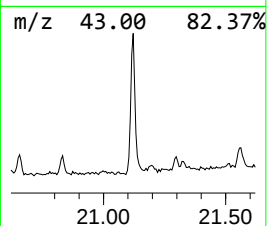
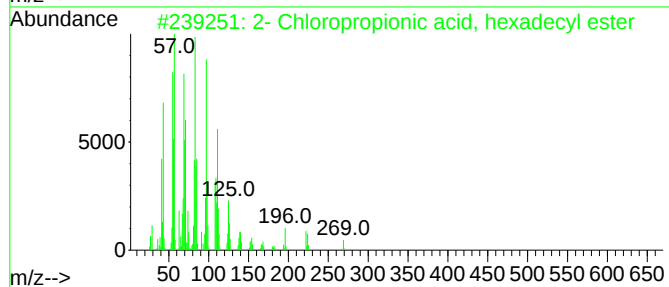
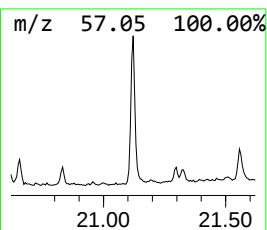
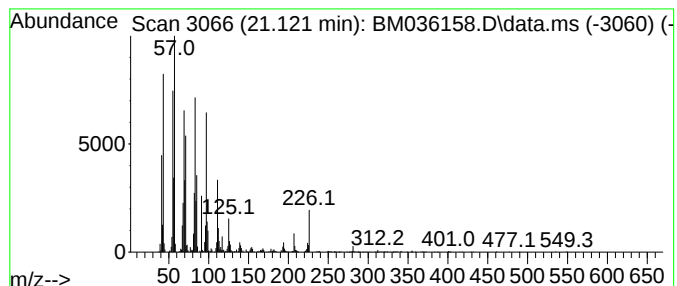
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Peak Number 3 2- Chloropropionic acid, he... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.121	8.18 ng	1388260	Chrysene-d12	21.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	94	
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93		
3	Cyclohexadecane	224	C16H32	000295-65-8	93		
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	89		
5	Cyclotetracosane	336	C24H48	000297-03-0	87		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.946	3.8	ng	287696	1	7.845	1530670	20.0
n-Hexadecanoic ...	18.127	5.0	ng	695423	4	17.227	2780300	20.0
2-Chloropropio...	21.121	8.2	ng	1388260	5	21.403	3393260	20.0