

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101421\
 Data File : BF125848.D
 Acq On : 14 Oct 2021 17:03
 Operator : JU/CG
 Sample : M4059-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SH-SUMP

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_F\METHODS\8270-BF100721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125848.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.445	567	571	575	rBV	2578259	2428361	42.05%	7.926%
2	6.451	738	742	745	rBV	1800315	1595444	27.63%	5.208%
3	6.834	803	807	810	rBV	1285327	1003251	17.37%	3.275%
4	7.392	897	902	905	rBV	2939716	3130496	54.20%	10.218%
5	8.016	1004	1008	1020	rBV	503908	449579	7.78%	1.467%
6	8.110	1020	1024	1028	rBV	1480162	1381460	23.92%	4.509%
7	9.192	1202	1208	1211	rBV	5758997	5775331	100.00%	18.851%
8	9.863	1318	1322	1326	rBV	1814562	1564405	27.09%	5.106%
9	10.651	1452	1456	1460	rBV	3481190	3490425	60.44%	11.393%
10	11.345	1571	1574	1578	rBV	1776851	1533597	26.55%	5.006%
11	11.874	1659	1664	1668	rBV	261601	261931	4.54%	0.855%
12	12.657	1794	1797	1805	rBV	123793	141758	2.45%	0.463%
13	12.933	1839	1844	1847	rBV	5572870	5489174	95.05%	17.917%
14	13.457	1930	1933	1938	rBV	78913	67333	1.17%	0.220%
15	13.833	1990	1997	2007	rBV2	81757	148559	2.57%	0.485%
16	13.980	2016	2022	2025	rBV	1277234	1086828	18.82%	3.548%
17	15.433	2263	2269	2273	rBV	883967	1088475	18.85%	3.553%

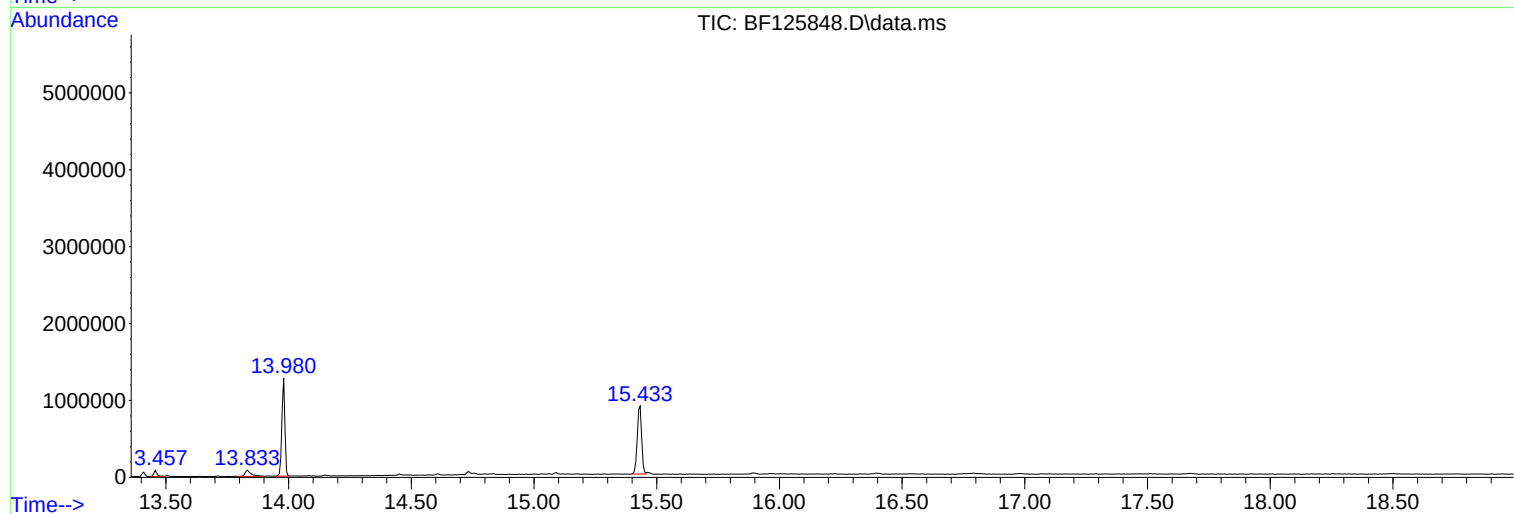
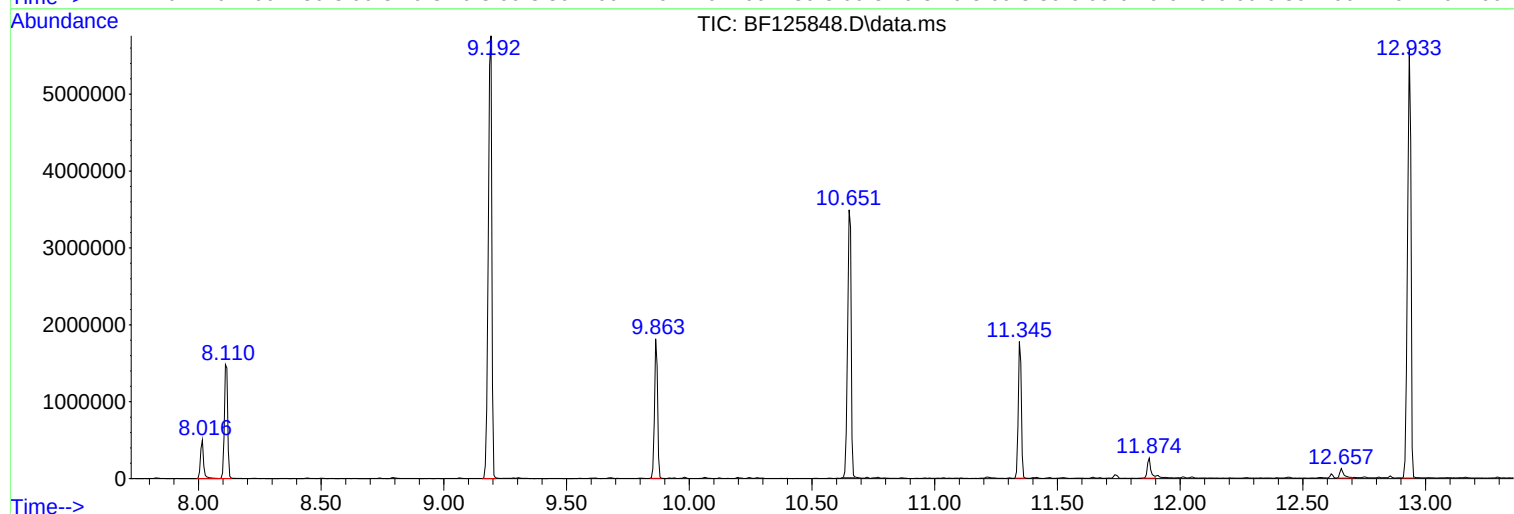
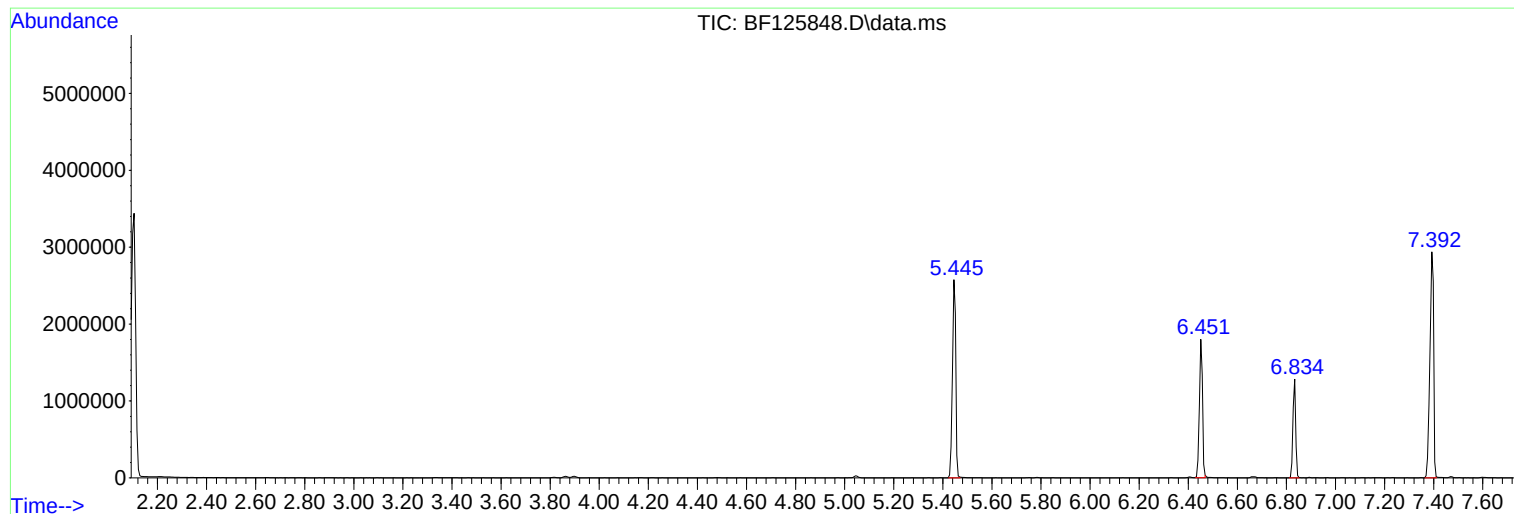
Sum of corrected areas: 30636407

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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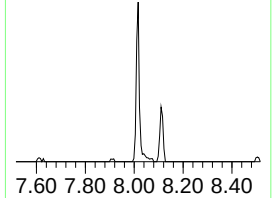
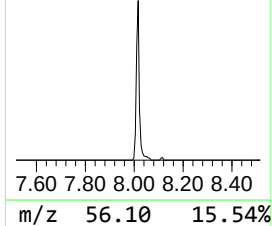
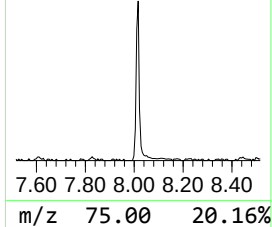
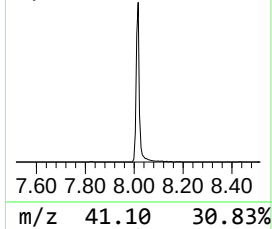
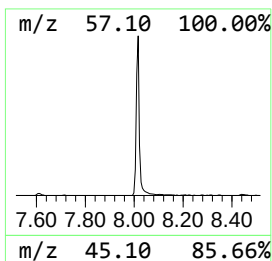
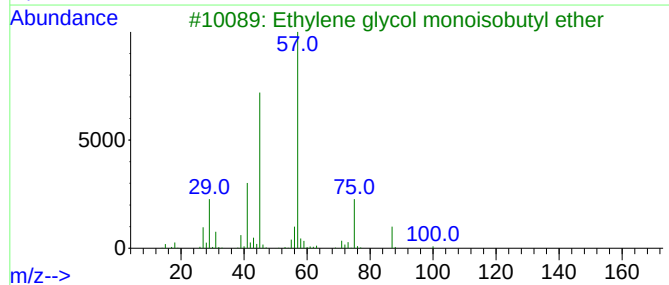
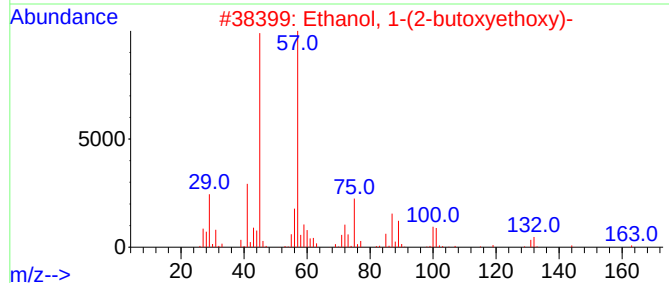
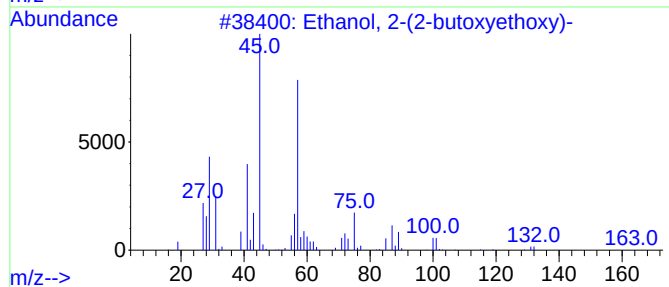
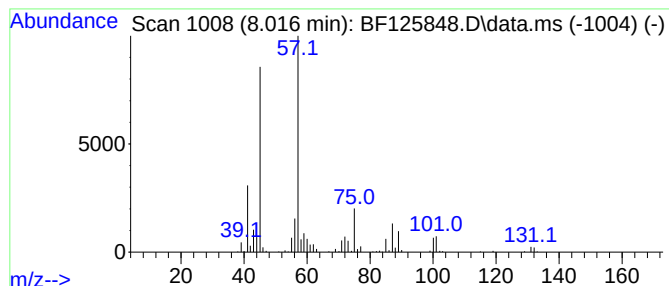
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.016	6.51 ng	449579	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	50
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



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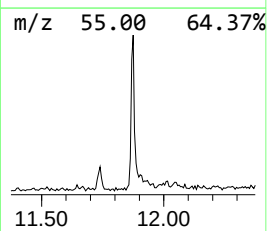
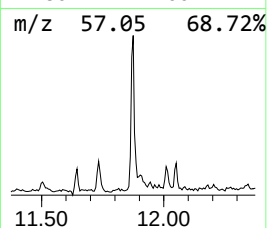
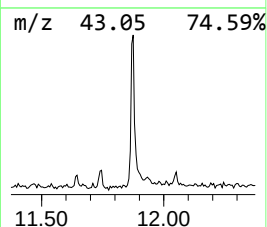
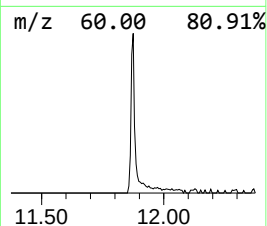
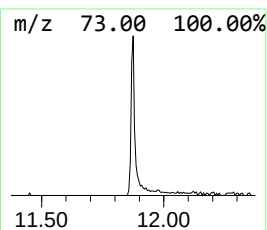
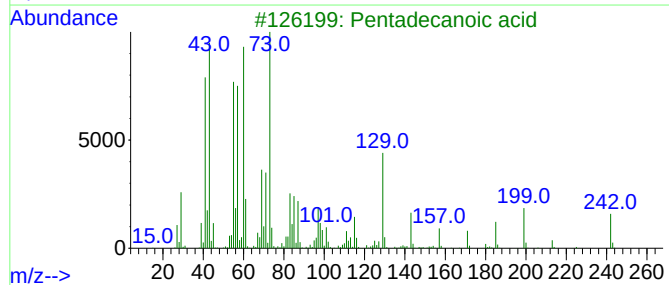
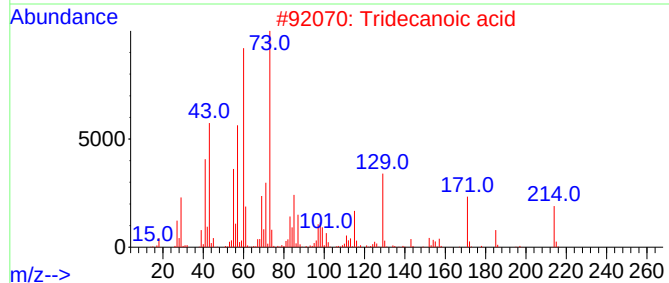
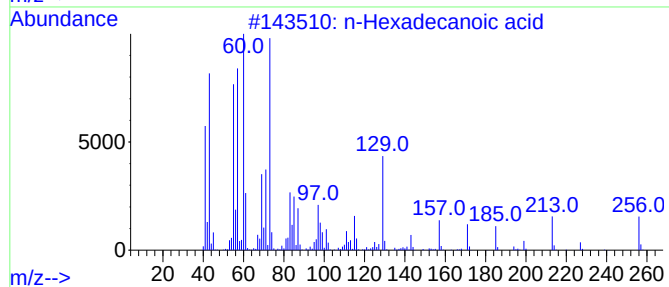
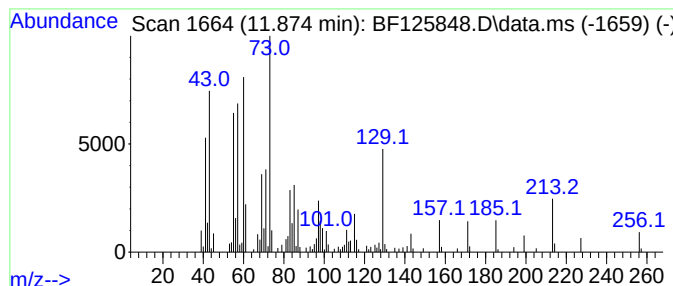
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	3.42 ng	261931	Phenanthrene-d10	11.345

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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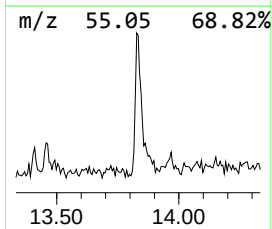
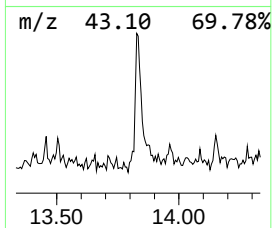
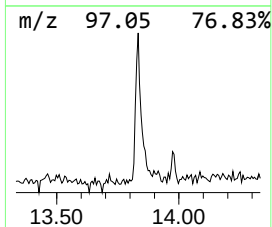
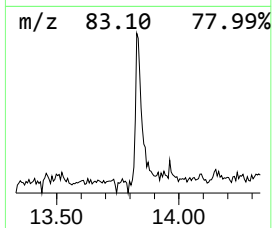
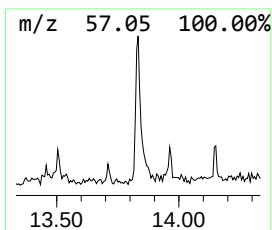
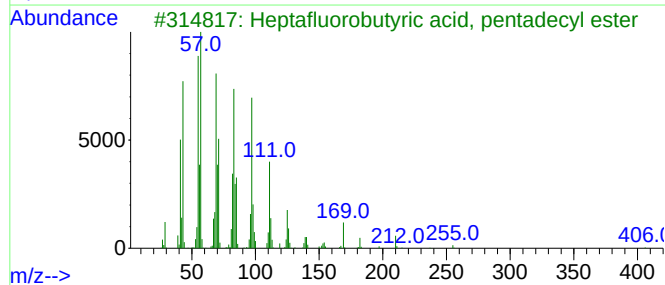
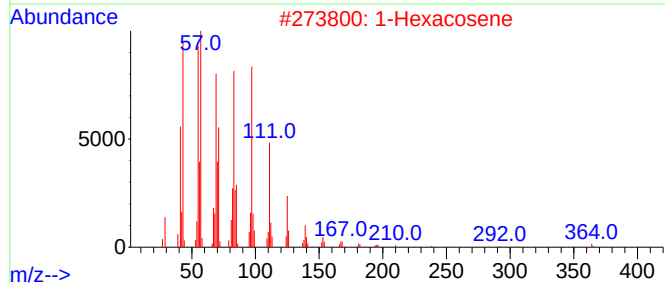
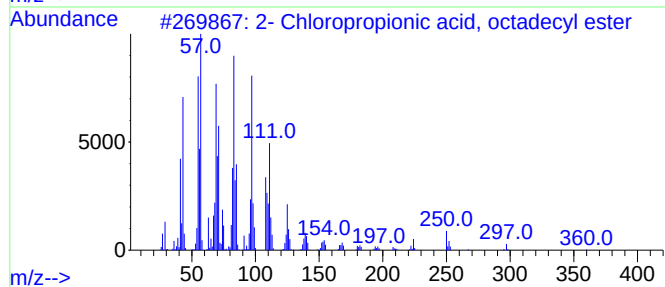
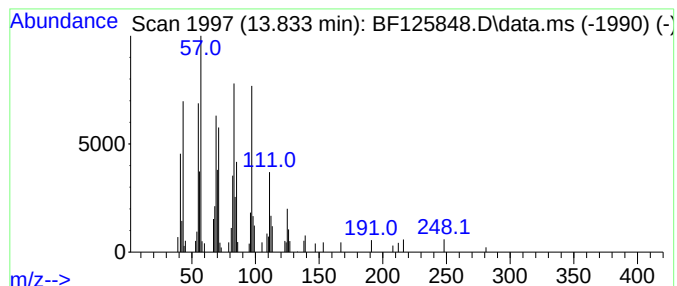
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Peak Number 3 2- Chloropropionic acid, oc... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	2.73 ng	148559	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94	
2	1-	Hexacosene	364	C26H52	018835-33-1	93	
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93		
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91		
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	8.016	6.5	ng	449579	2	8.116	1381460	20.0
n-Hexadecanoic ...	11.874	3.4	ng	261931	4	11.345	1533600	20.0
2- Chloropropio...	13.833	2.7	ng	148559	5	13.980	1086830	20.0