

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040422\
 Data File : BG053019.D
 Acq On : 4 Apr 2022 22:17
 Operator : CG/JU
 Sample : N2207-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20220352-AMENDED-098-21-01

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_G\Methods\8270-BG031522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053019.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.226	305	313	326	rVB	1228619	1970999	100.00%	20.699%
2	5.690	385	392	401	rBV	54536	89074	4.52%	0.935%
3	7.276	654	662	675	rBV	257391	457072	23.19%	4.800%
4	8.128	798	807	814	rBV2	125831	215141	10.92%	2.259%
5	9.286	996	1004	1012	rBV	329114	592290	30.05%	6.220%
6	9.650	1058	1066	1074	rBV2	55227	108568	5.51%	1.140%
7	10.936	1275	1285	1293	rBV	160853	297859	15.11%	3.128%
8	13.374	1692	1700	1706	rBV	785279	1237545	62.79%	12.997%
9	13.497	1714	1721	1728	rVB2	16058	29631	1.50%	0.311%
10	14.749	1926	1934	1941	rVB	271328	427250	21.68%	4.487%
11	15.712	2092	2098	2104	rBV2	16607	26127	1.33%	0.274%
12	16.229	2179	2186	2192	rBV4	52131	84869	4.31%	0.891%
13	16.458	2215	2225	2231	rBV	32385	52191	2.65%	0.548%
14	17.486	2394	2400	2407	rBV	346210	548717	27.84%	5.763%
15	18.144	2508	2512	2516	rVB	20094	24894	1.26%	0.261%
16	19.901	2806	2811	2818	rVB	31251	48769	2.47%	0.512%
17	20.089	2837	2843	2849	rBV	1464045	1930957	97.97%	20.279%
18	21.399	3061	3066	3075	rBV3	64683	107371	5.45%	1.128%
19	21.774	3123	3130	3138	rVB	361486	617999	31.35%	6.490%
20	22.603	3266	3271	3276	rVB9	14052	28054	1.42%	0.295%
21	25.076	3681	3692	3702	rBV3	201942	626593	31.79%	6.580%

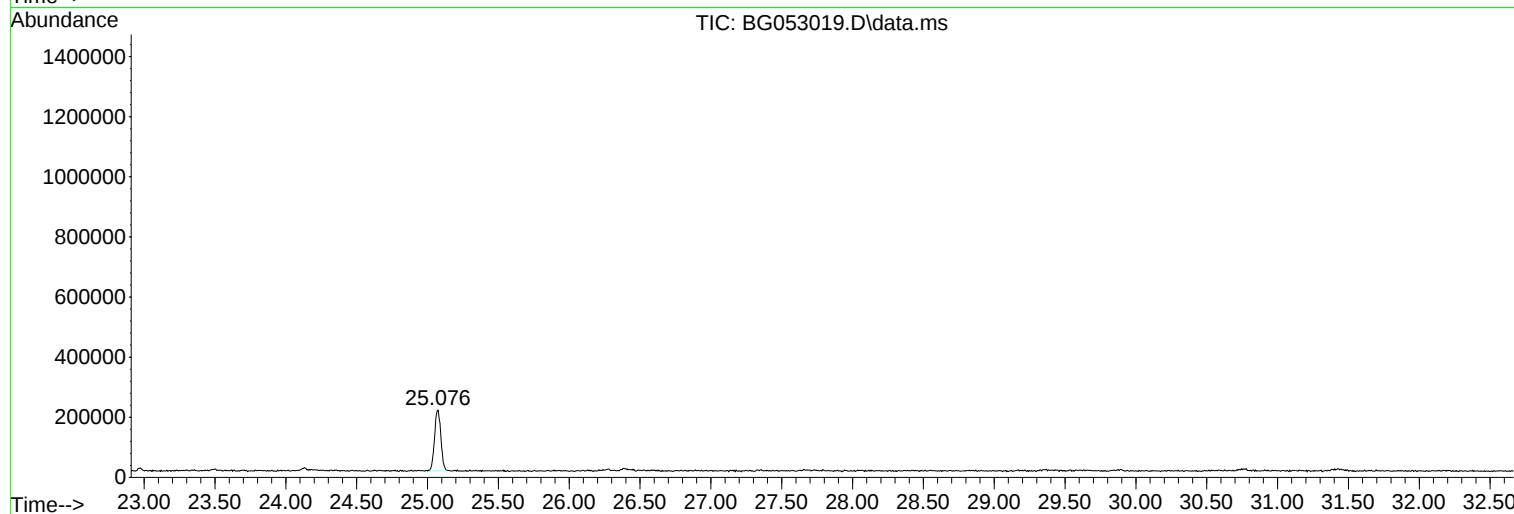
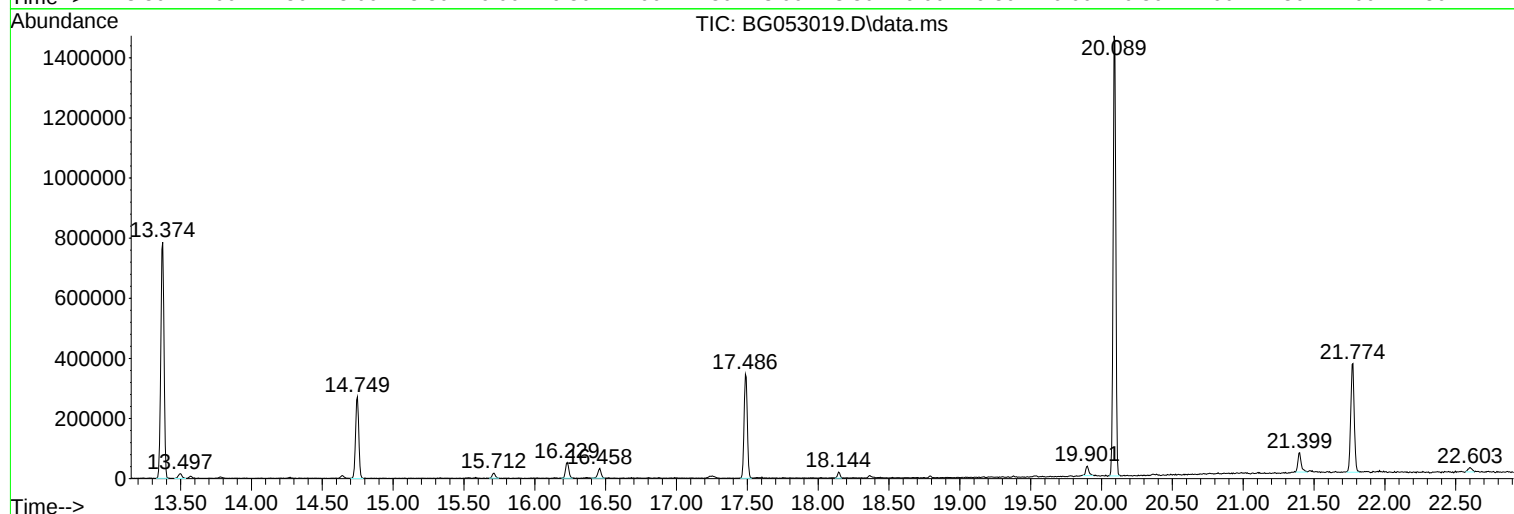
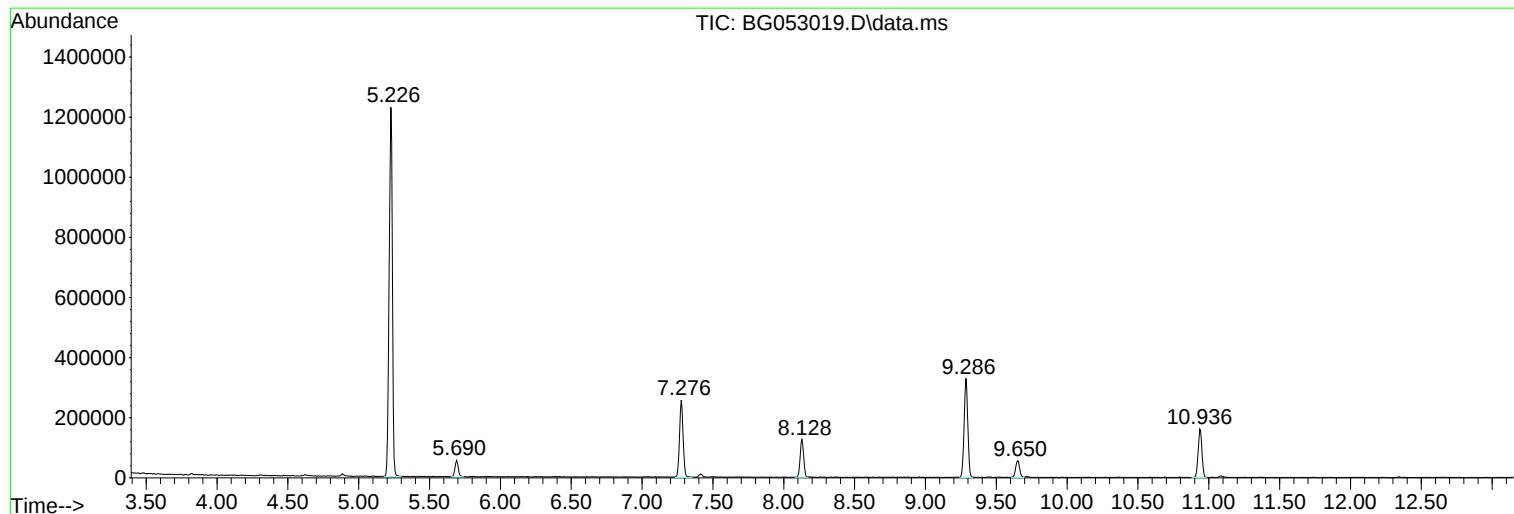
Sum of corrected areas: 9521970

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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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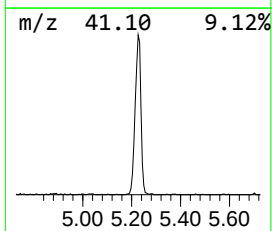
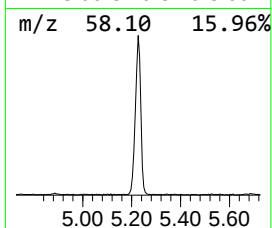
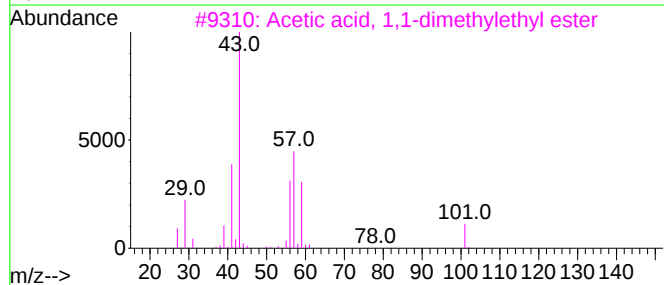
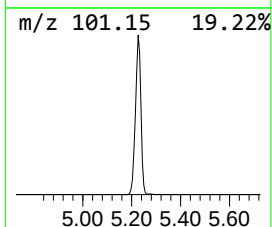
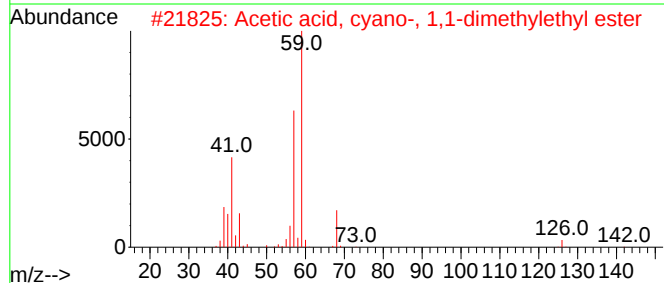
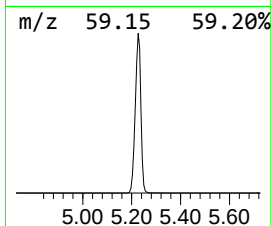
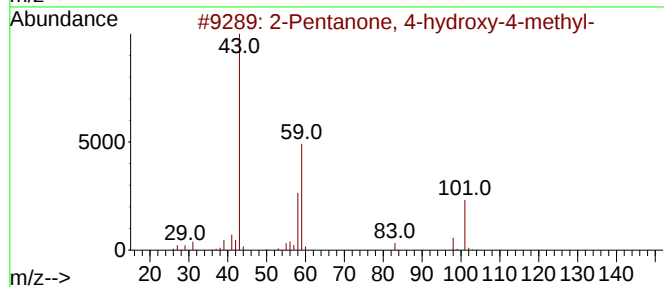
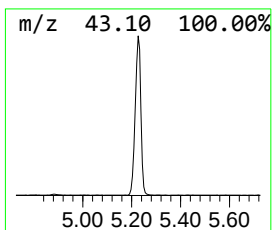
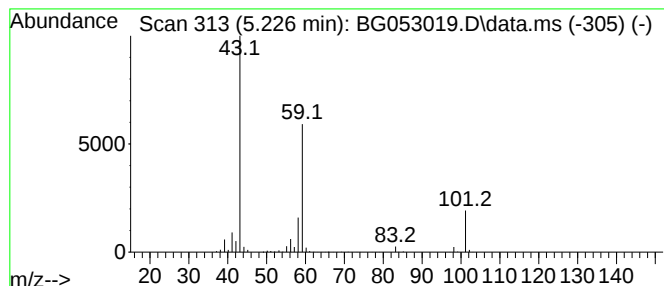
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.226	183.23 ng	1971000	1,4-Dichlorobenzene-d4	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12		



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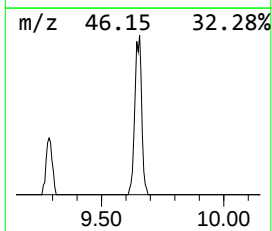
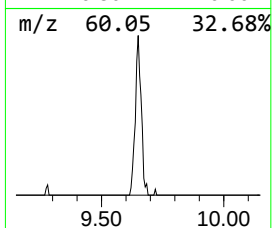
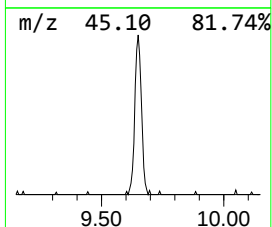
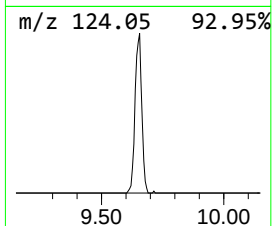
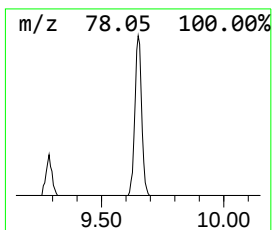
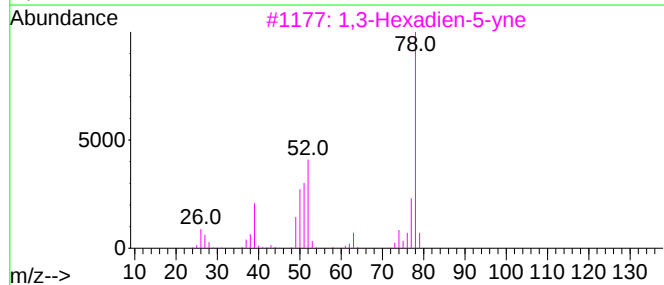
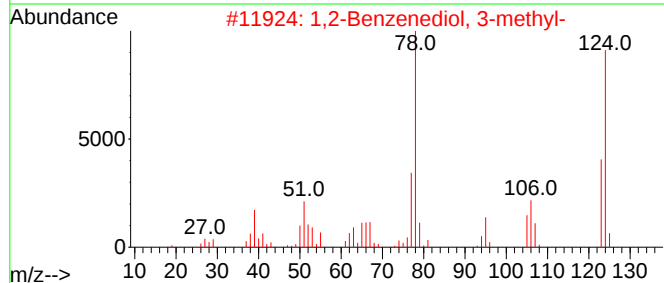
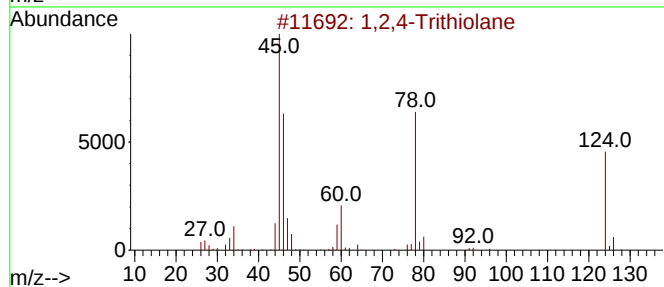
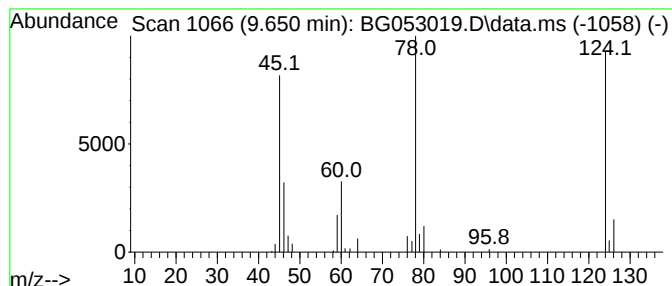
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Peak Number 2 1,2,4-Trithiolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.650	7.29 ng	108568	Naphthalene-d8	10.936

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	91
2			1,2-Benzenediol, 3-methyl-	124	C7H8O2	000488-17-5	42
3			1,3-Hexadien-5-yne	78	C6H6	010420-90-3	25
4			Benzene	78	C6H6	000071-43-2	9
5			1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	9



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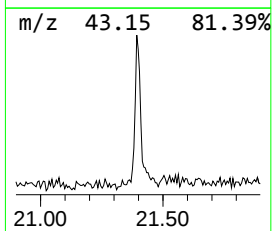
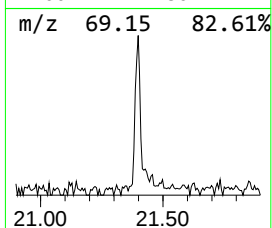
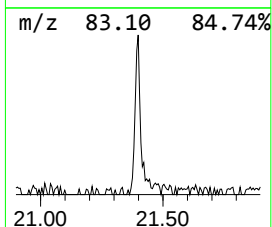
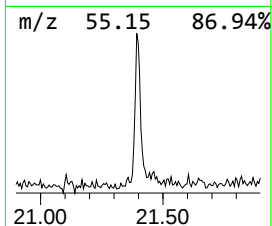
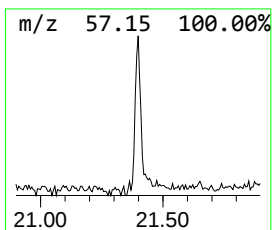
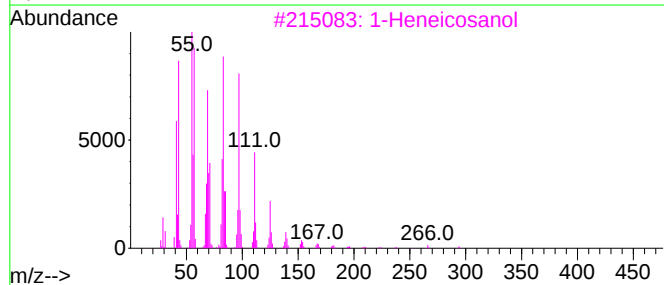
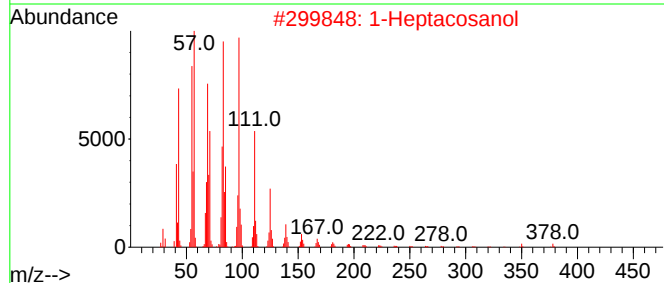
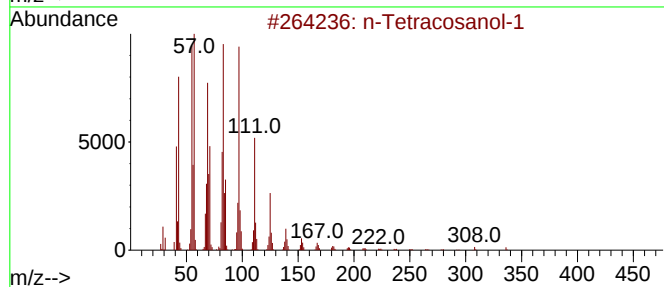
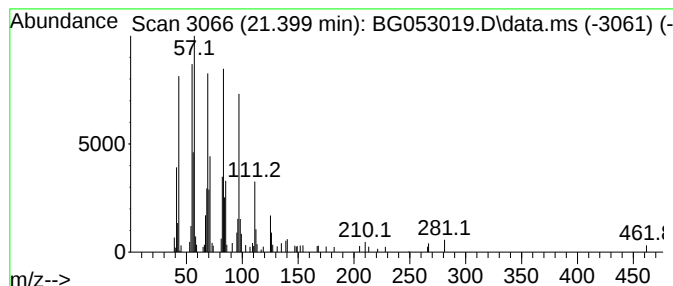
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Peak Number 3 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.398	3.47 ng	107371	Chrysene-d12	21.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2			1-Heptacosanol	396	C27H56O	002004-39-9	91
3			1-Heneicosanol	312	C21H44O	015594-90-8	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.226	183.2	ng	1971000	1	8.128	215141	20.0
1,2,4-Trithiolane	9.650	7.3	ng	108568	2	10.936	297859	20.0
n-Tetracosanol-1	21.398	3.5	ng	107371	5	21.769	617999	20.0