

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
 Data File : BM028577.D
 Acq On : 27 Jan 2021 19:45
 Operator : CG/JU
 Sample : M1236-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 2922

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-BM012021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028577.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.522	391	397	406	rBB	394023	576089	64.91%	9.684%
2	7.169	670	677	688	rBV	375296	616927	69.51%	10.370%
3	7.969	807	813	819	rBB	90779	140934	15.88%	2.369%
4	9.140	1005	1012	1025	rVB	231256	377313	42.52%	6.343%
5	10.781	1284	1291	1299	rBV	121939	194725	21.94%	3.273%
6	13.233	1702	1708	1717	rBV	498471	719988	81.13%	12.103%
7	14.063	1844	1849	1855	rBV	7258	9378	1.06%	0.158%
8	14.610	1937	1942	1949	rBV2	161714	237130	26.72%	3.986%
9	16.098	2189	2195	2204	rBV	413947	566409	63.82%	9.521%
10	17.345	2401	2407	2411	rBV	195045	261831	29.50%	4.401%
11	17.386	2411	2414	2421	rVB2	9713	14178	1.60%	0.238%
12	18.221	2551	2556	2566	rBV	84882	128468	14.48%	2.160%
13	18.710	2634	2639	2645	rBV	10043	16870	1.90%	0.284%
14	18.974	2679	2684	2689	rBV	65169	79660	8.98%	1.339%
15	19.062	2695	2699	2705	rBV	18449	24653	2.78%	0.414%
16	19.127	2706	2710	2715	rBV4	7164	11232	1.27%	0.189%
17	19.380	2749	2753	2758	rBV	35215	45276	5.10%	0.761%
18	19.492	2768	2772	2781	rBV2	42830	73363	8.27%	1.233%
19	19.604	2787	2791	2794	rBV	18287	21114	2.38%	0.355%
20	19.745	2811	2815	2821	rVB	29535	39981	4.50%	0.672%
21	19.939	2843	2848	2856	rBV	718041	887482	100.00%	14.918%
22	20.127	2878	2880	2885	rVB	8031	9486	1.07%	0.159%
23	20.574	2953	2956	2959	rBV2	23147	26044	2.93%	0.438%
24	20.609	2959	2962	2968	rVB	14077	20959	2.36%	0.352%
25	20.809	2993	2996	3001	rBV	43269	50522	5.69%	0.849%
26	21.180	3055	3059	3067	rBV	113999	147671	16.64%	2.482%
27	21.480	3105	3110	3114	rBV	252286	330468	37.24%	5.555%
28	23.745	3490	3495	3502	rVB2	174896	320801	36.15%	5.393%

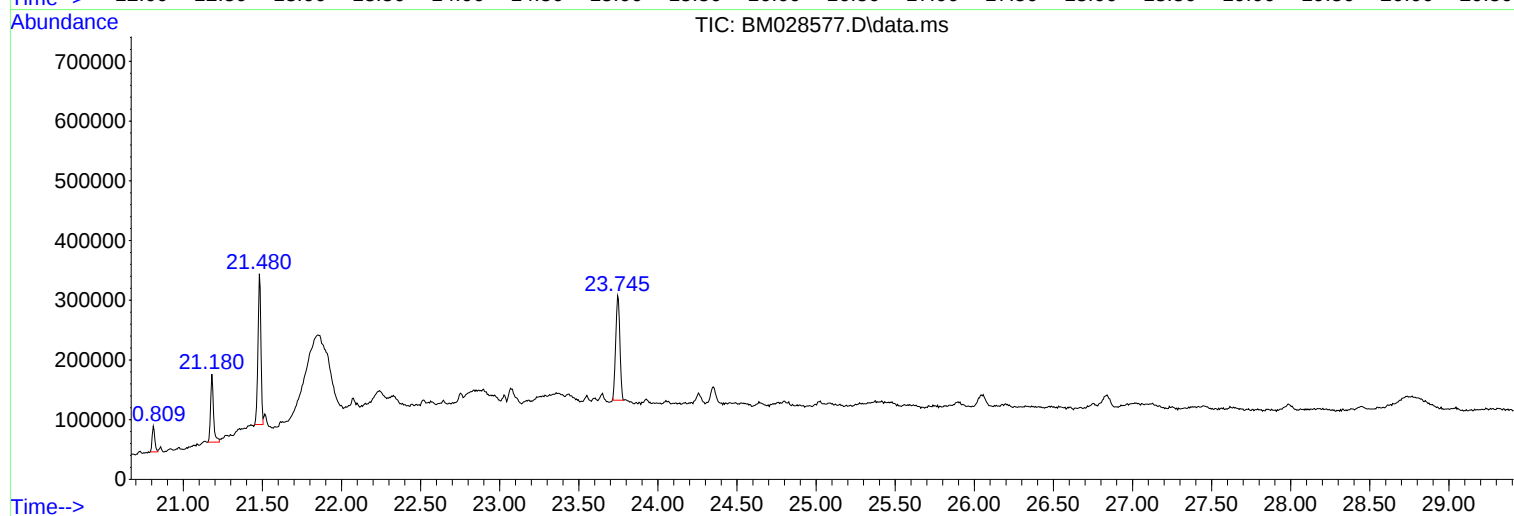
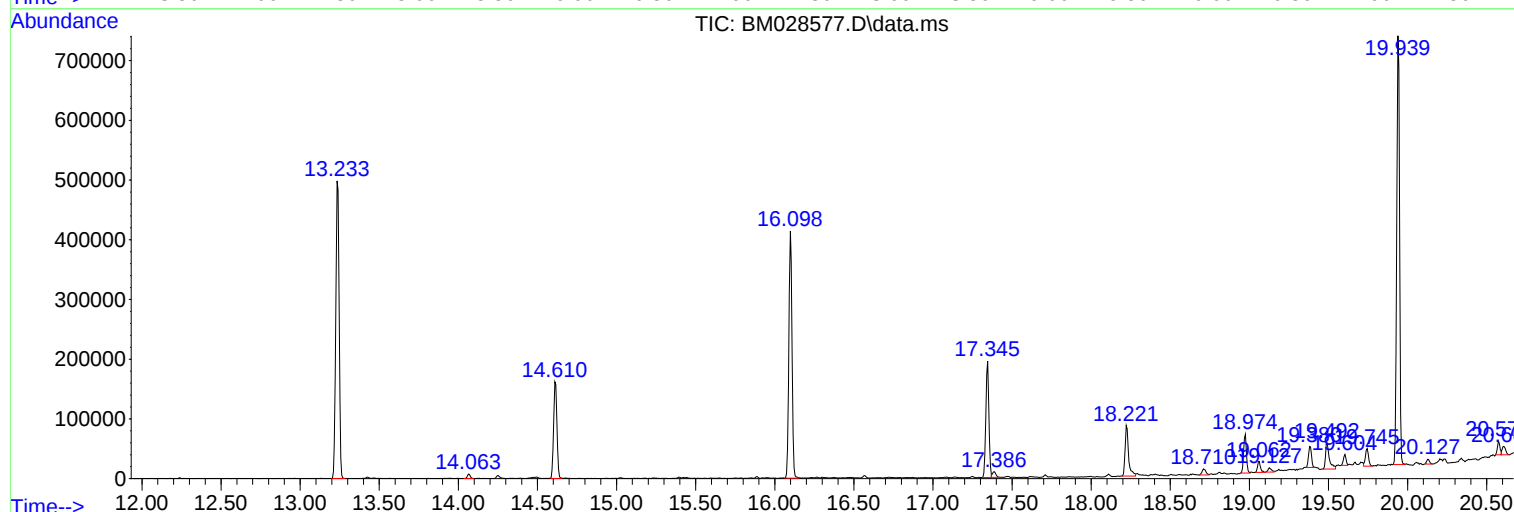
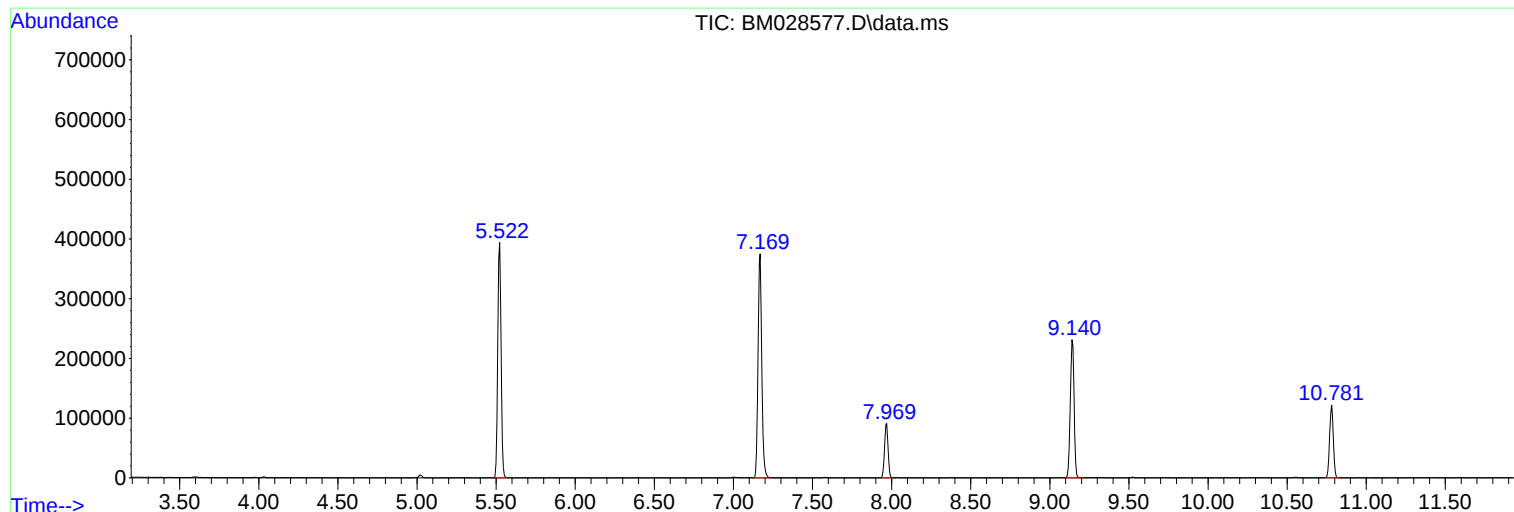
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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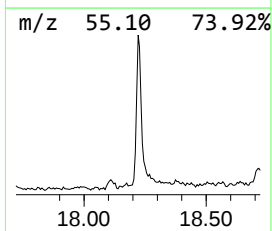
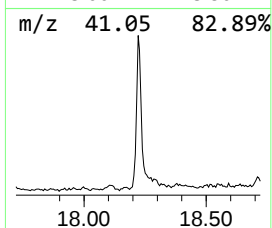
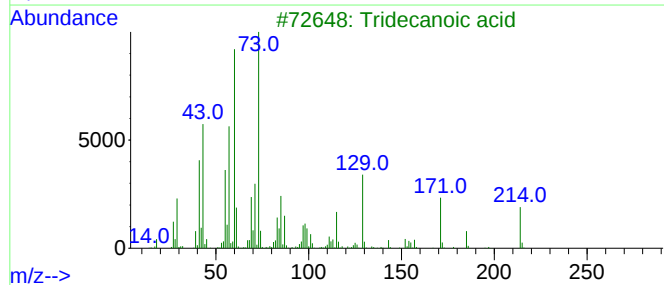
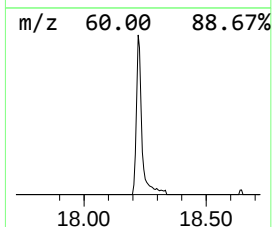
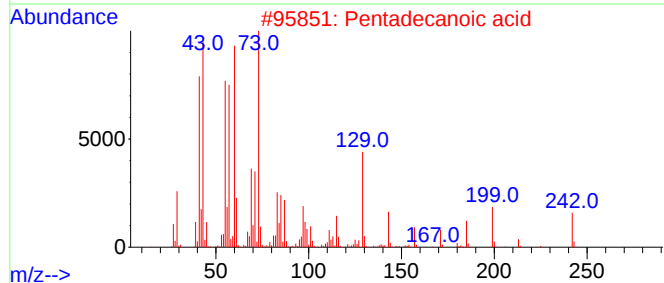
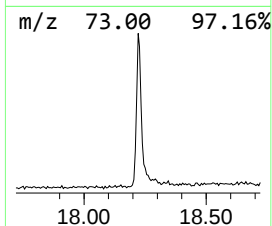
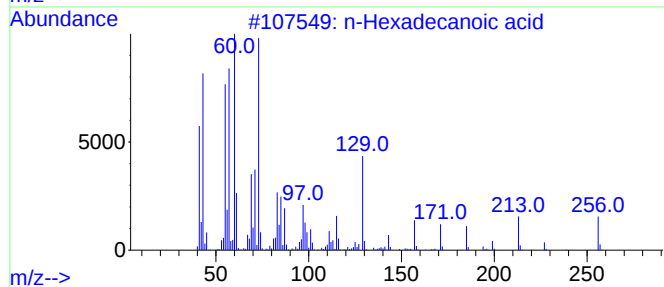
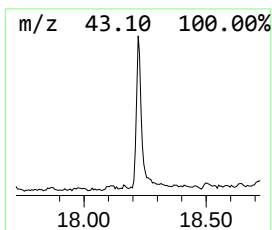
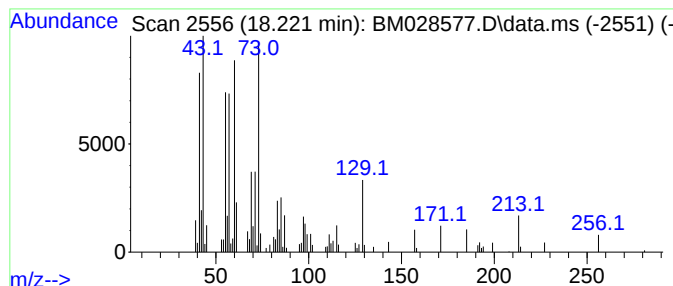
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.221	9.81 ng	128468	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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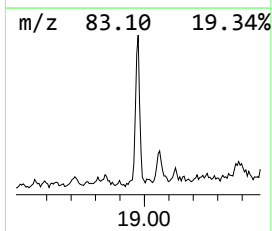
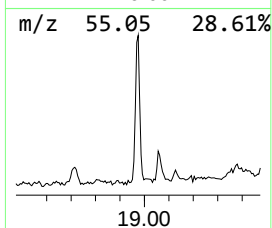
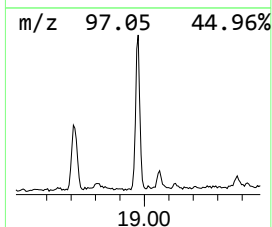
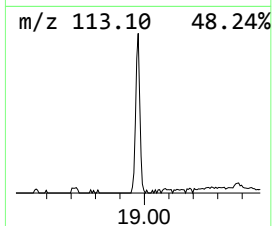
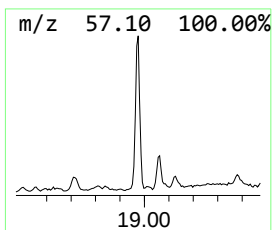
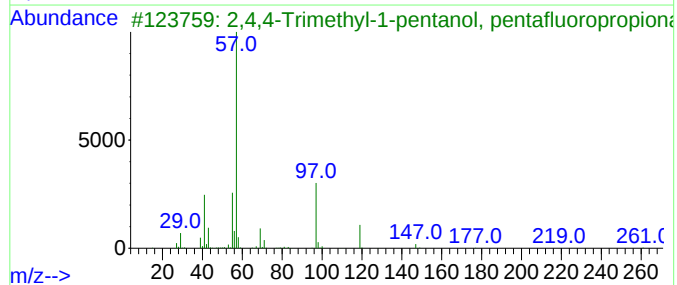
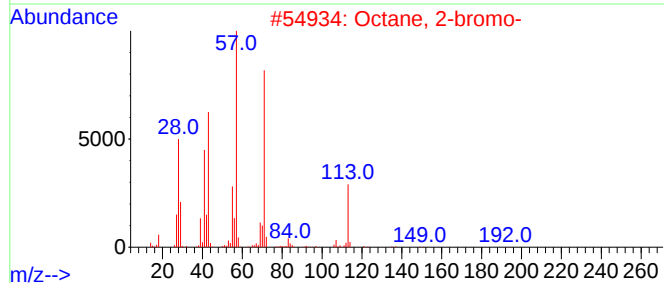
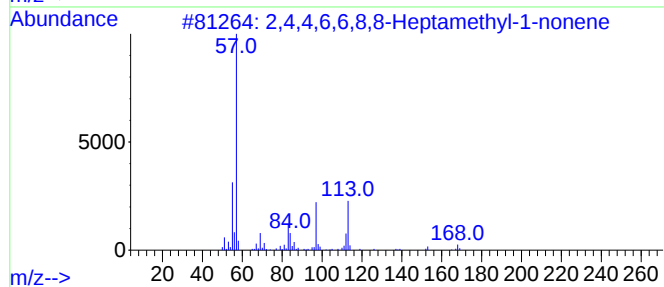
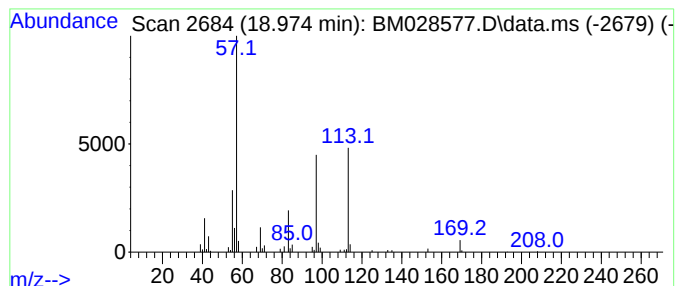
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown18.974 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.974	6.08 ng	79660	Phenanthrene-d10	17.345

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	40
2		Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
3		2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
4		1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28
5		Hexanal, 3,5,5-trimethyl-	142	C9H18O	005435-64-3	27



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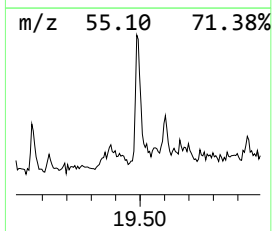
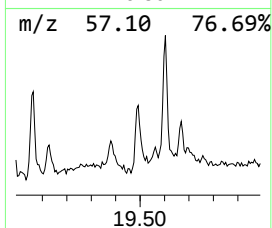
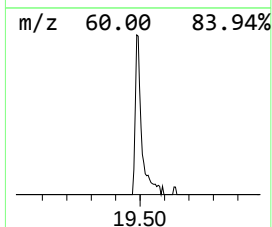
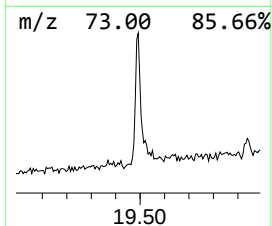
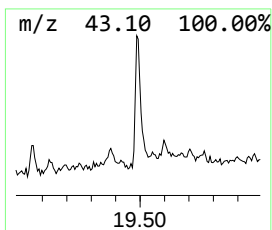
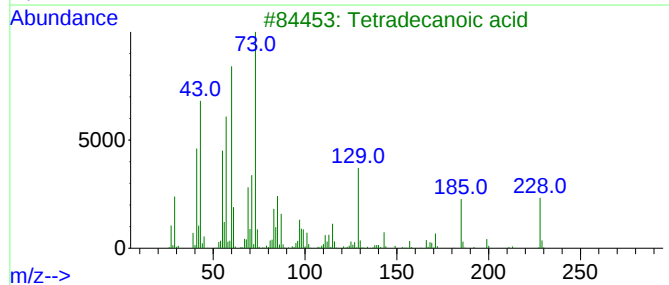
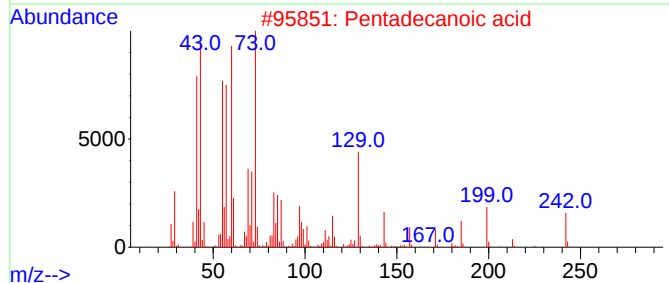
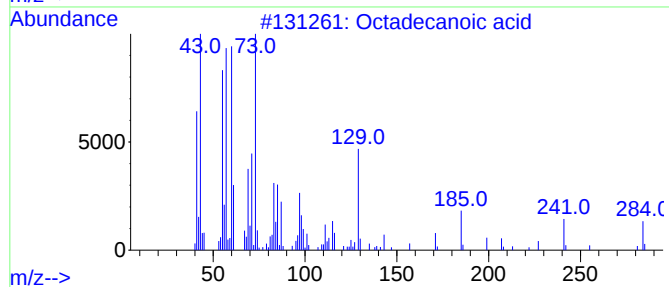
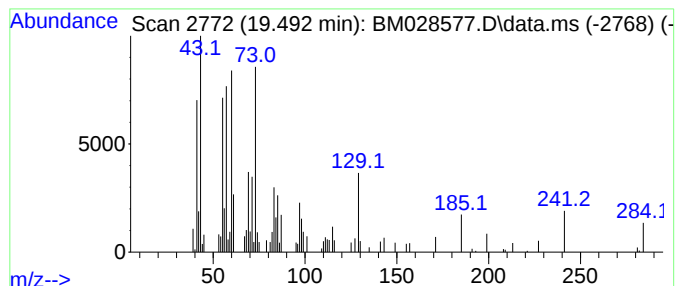
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.492	4.44 ng	73363	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	59
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Undecanoic acid	186	C11H22O2	000112-37-8	50
5			Lactose	342	C12H22O11	000063-42-3	50



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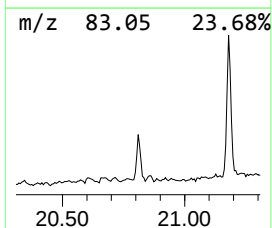
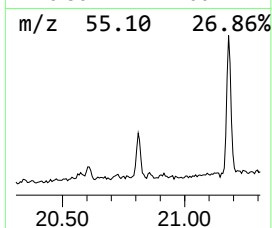
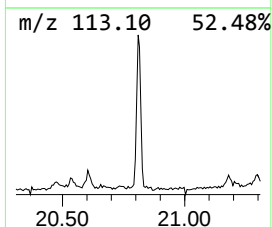
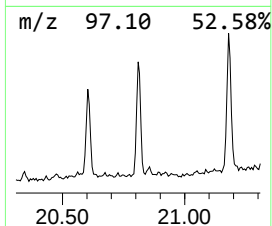
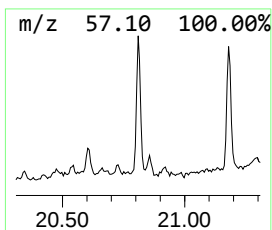
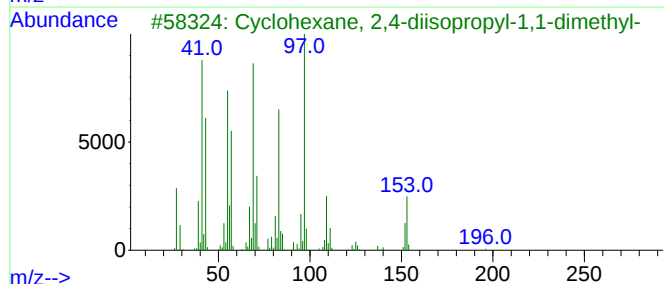
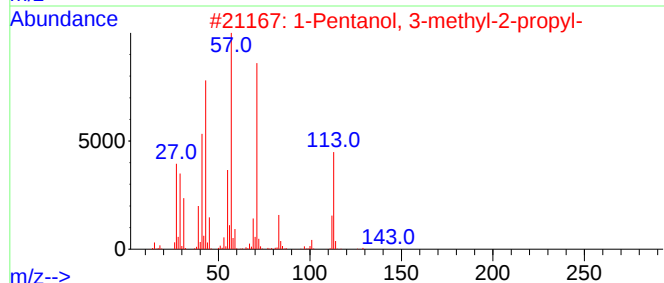
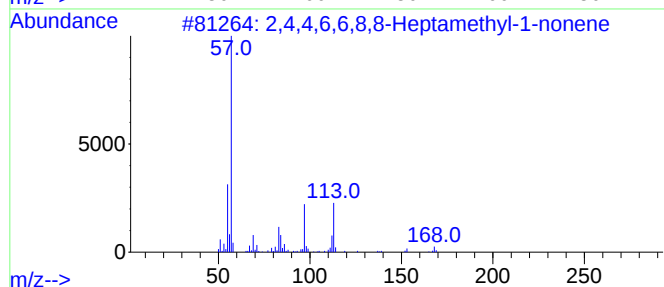
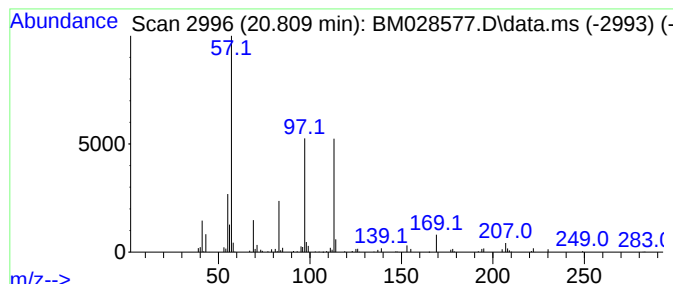
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Peak Number 4 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.809	3.06 ng	50522	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	64		
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	38		
3	Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	16		
4	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	16		
5	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	16		



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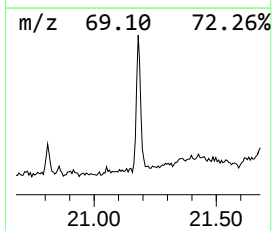
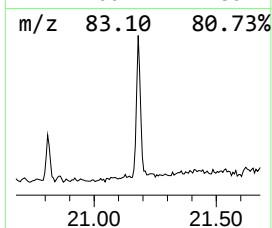
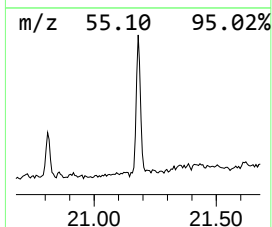
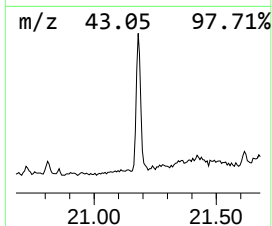
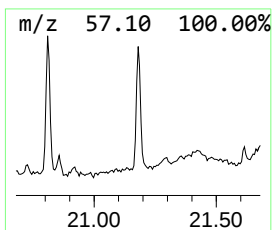
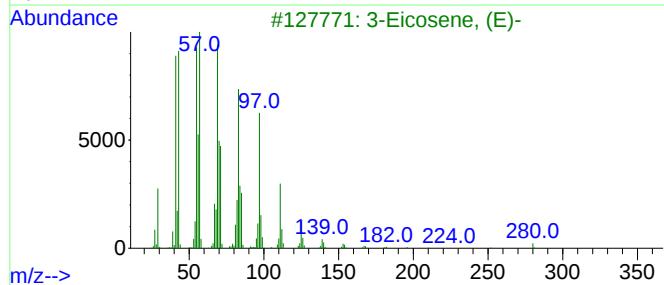
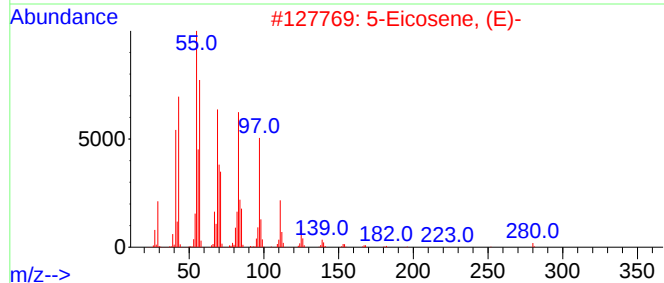
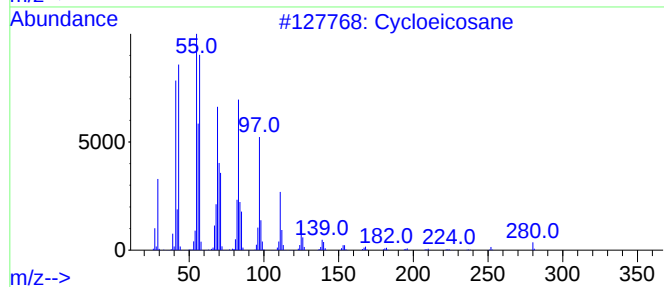
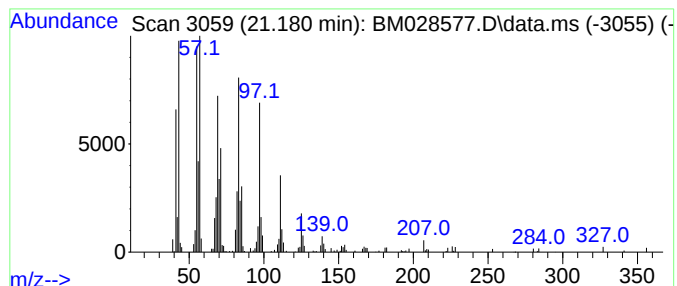
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Peak Number 5 Cycloeicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	8.94 ng	147671	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	97
2			5-Eicosene, (E)-	280	C20H40	074685-30-6	96
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.221	9.8	ng	128468	4	17.345	261831	20.0
unknown18.974	18.974	6.1	ng	79660	4	17.345	261831	20.0
Octadecanoic acid	19.492	4.4	ng	73363	5	21.480	330468	20.0
2,4,4,6,6,8,8-H...	20.809	3.1	ng	50522	5	21.480	330468	20.0
Cycloeicosane	21.180	8.9	ng	147671	5	21.480	330468	20.0