

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
 Data File : BM028574.D
 Acq On : 27 Jan 2021 17:56
 Operator : CG/JU
 Sample : M1236-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 J2288R-WO(N)-1-13-1

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: BM028574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.528	391	398	408	rBB	334209	504146	66.03%	9.969%
2	7.175	671	678	689	rBV	312067	529913	69.41%	10.478%
3	7.969	807	813	820	rBB	90233	139285	18.24%	2.754%
4	9.139	1006	1012	1019	rBV	202571	330821	43.33%	6.541%
5	10.780	1283	1291	1298	rVB	114908	187109	24.51%	3.700%
6	13.239	1702	1709	1715	rBV	438168	644468	84.41%	12.743%
7	14.615	1937	1943	1949	rBV	151967	223726	29.30%	4.424%
8	16.098	2190	2195	2204	rBV	323888	461084	60.39%	9.117%
9	17.345	2401	2407	2412	rBV	177220	237963	31.17%	4.705%
10	18.221	2551	2556	2565	rBV	80428	110308	14.45%	2.181%
11	18.715	2636	2640	2646	rVB	6170	9031	1.18%	0.179%
12	18.974	2679	2684	2688	rBV	42556	52631	6.89%	1.041%
13	19.062	2694	2699	2705	rBV	13987	17501	2.29%	0.346%
14	19.486	2767	2771	2779	rBV	35156	48158	6.31%	0.952%
15	19.603	2787	2791	2795	rBV	11726	13611	1.78%	0.269%
16	19.939	2843	2848	2853	rBV	636733	763465	100.00%	15.096%
17	20.133	2877	2881	2887	rVB3	6030	7993	1.05%	0.158%
18	20.603	2958	2961	2966	rBV	12139	15634	2.05%	0.309%
19	20.809	2992	2996	3001	rBV	44284	54181	7.10%	1.071%
20	20.856	3001	3004	3008	rVB	9621	12001	1.57%	0.237%
21	21.180	3055	3059	3064	rBV	104468	119911	15.71%	2.371%
22	21.480	3105	3110	3115	rBV	230614	277263	36.32%	5.482%
23	23.744	3489	3495	3503	rVB2	158145	297063	38.91%	5.874%

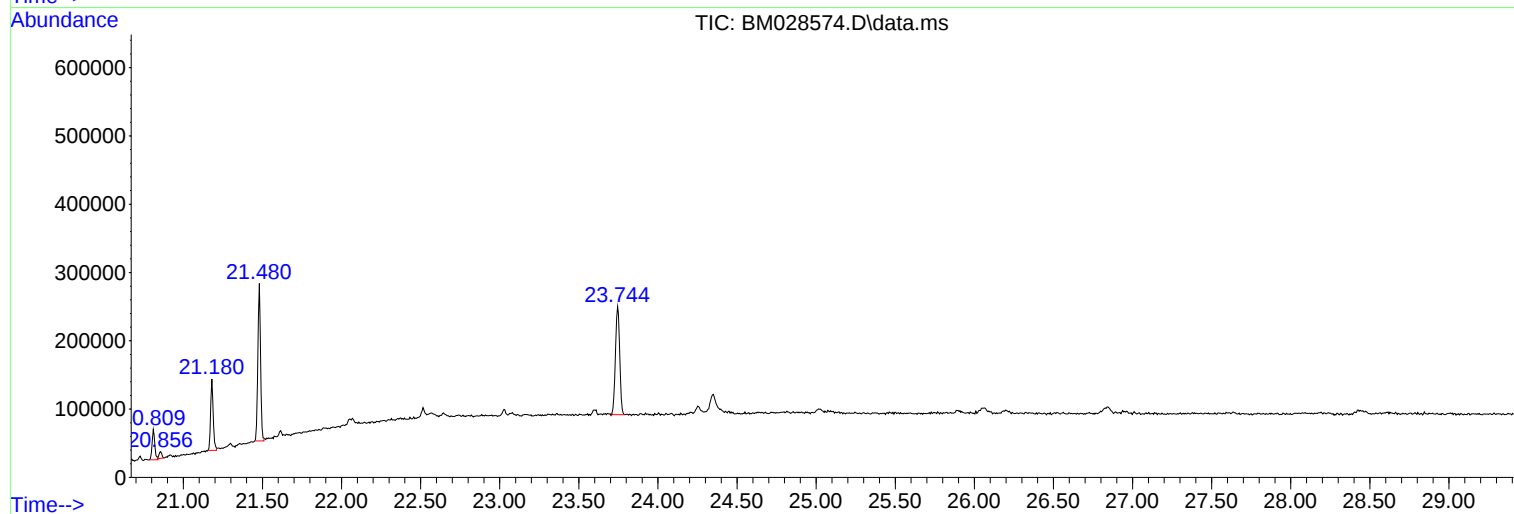
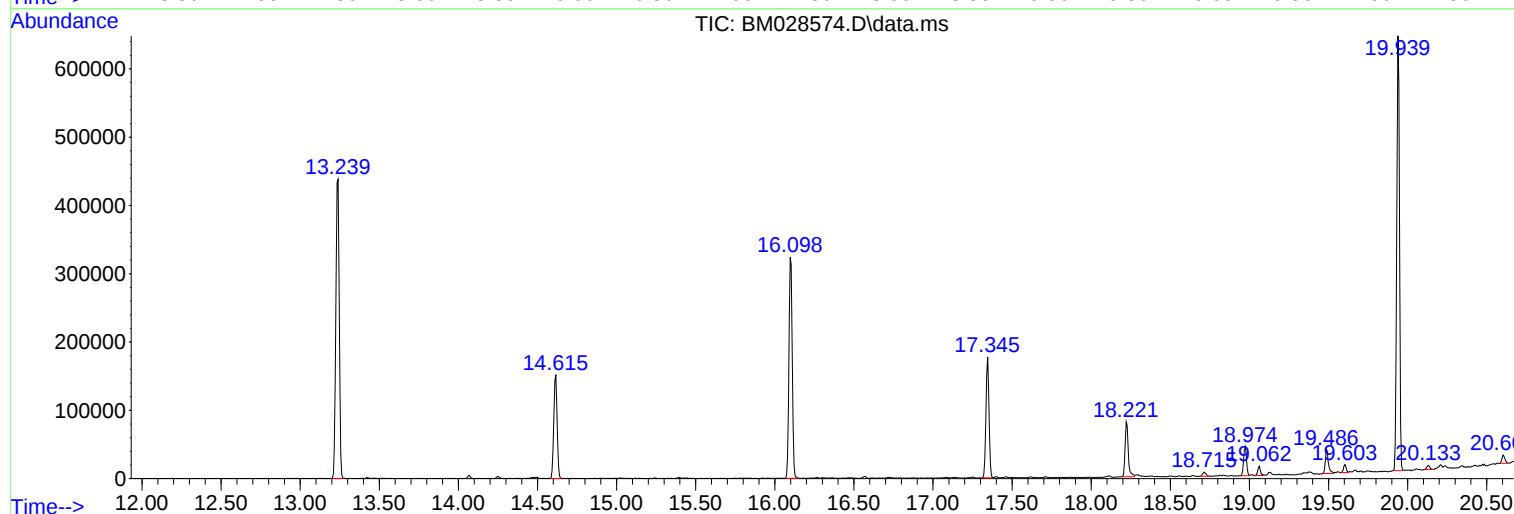
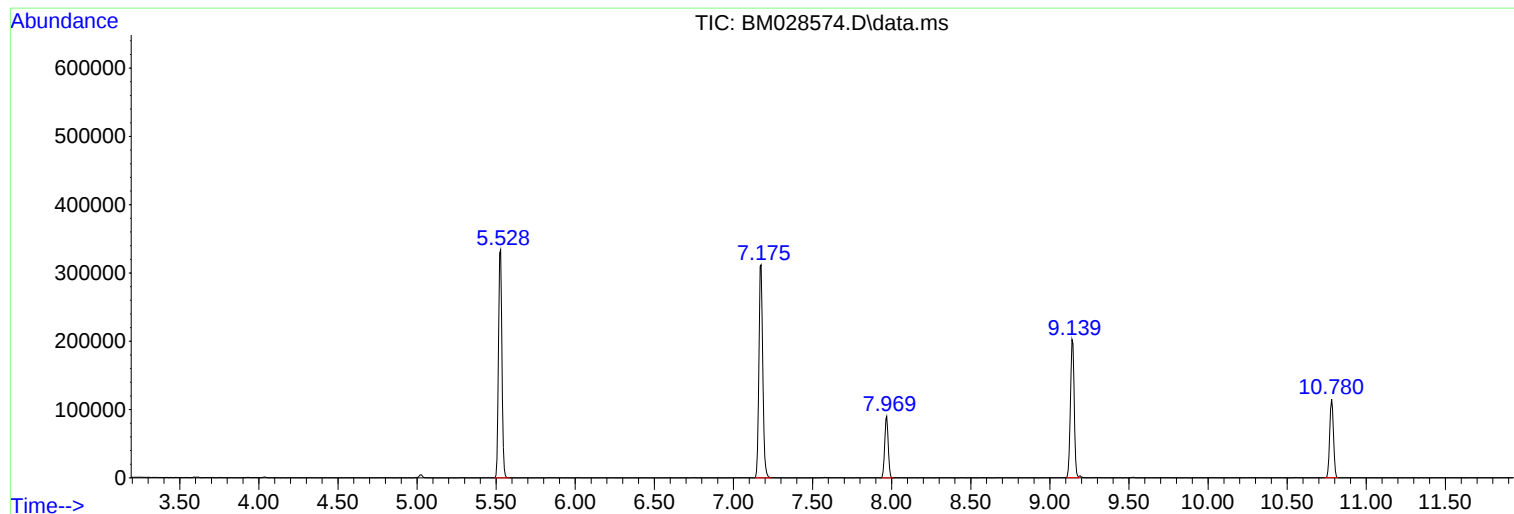
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Instrument :
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ClientSampleId :
J2288R-WO(N)-1-13-1

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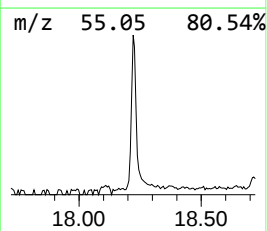
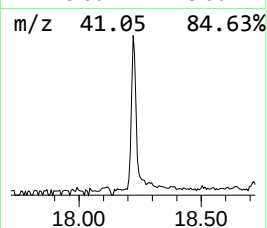
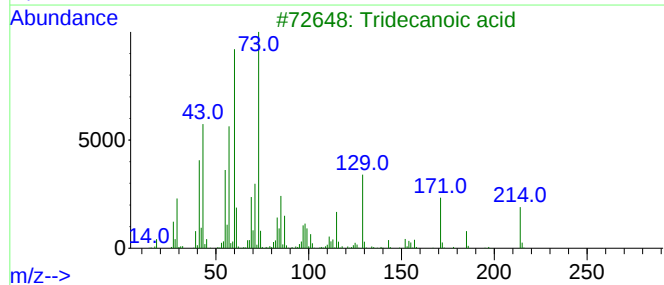
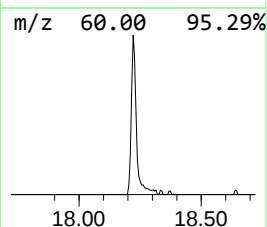
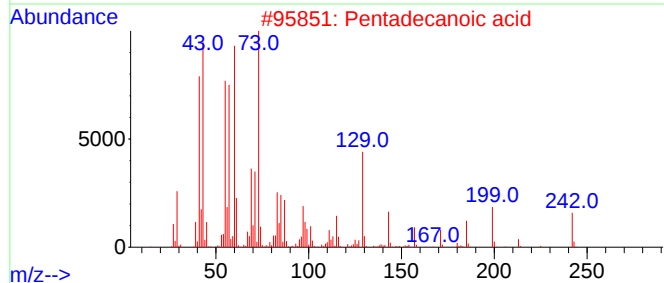
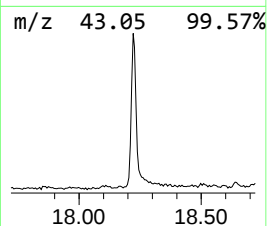
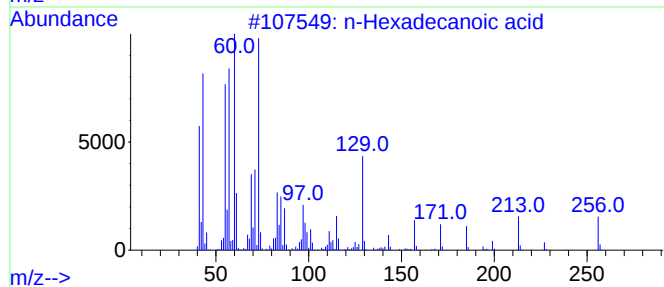
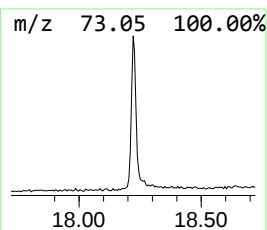
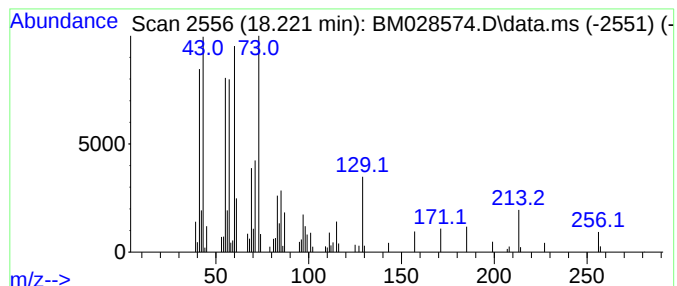
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	9.27 ng	110308	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	76
3			Tridecanoic acid	214	C13H26O2	000638-53-9	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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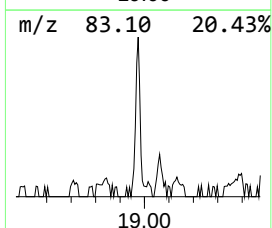
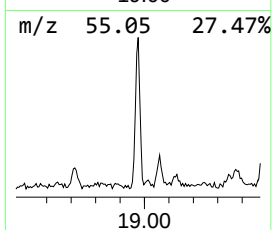
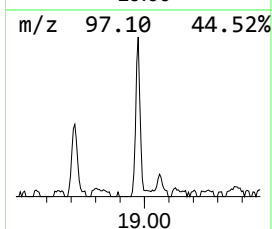
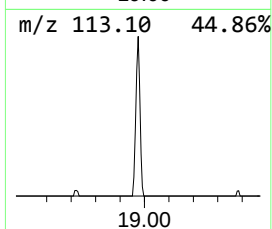
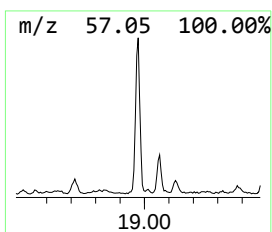
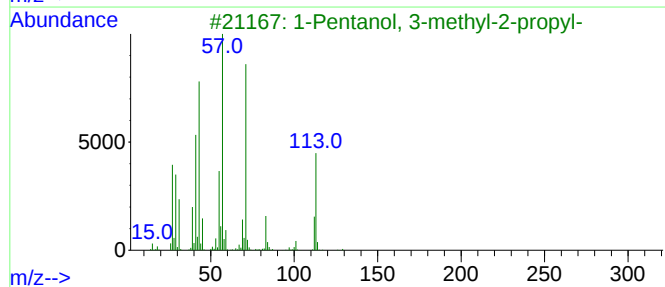
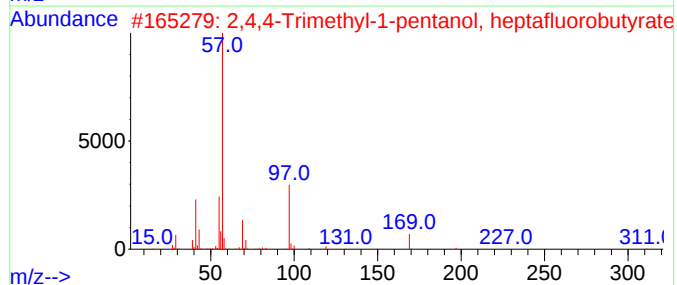
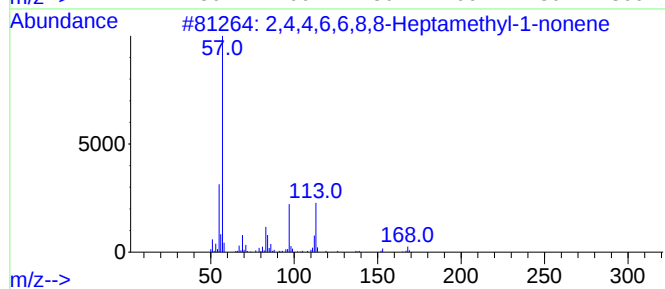
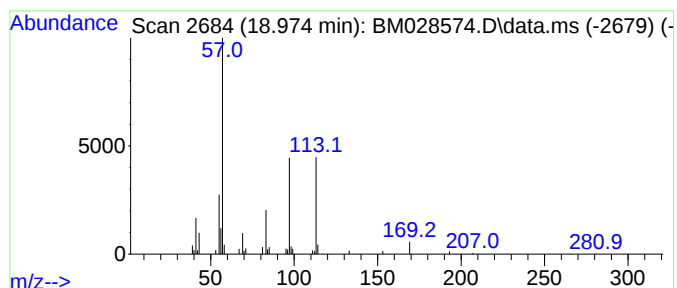
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown18.974 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.974	4.42 ng	52631	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	37
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2		1000365-01-4	32
3	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O		054004-40-9	28
4	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2		1000365-19-5	25
5	Octane, 2-bromo-	192	C8H17Br		000557-35-7	25



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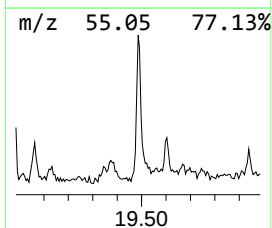
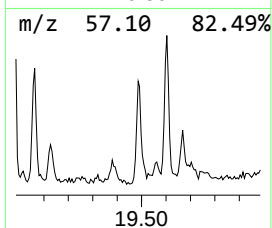
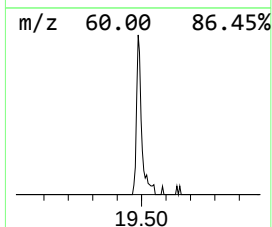
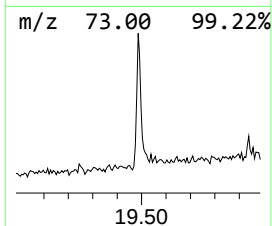
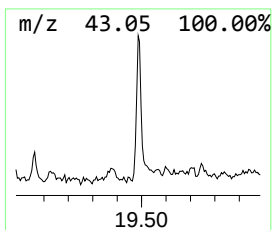
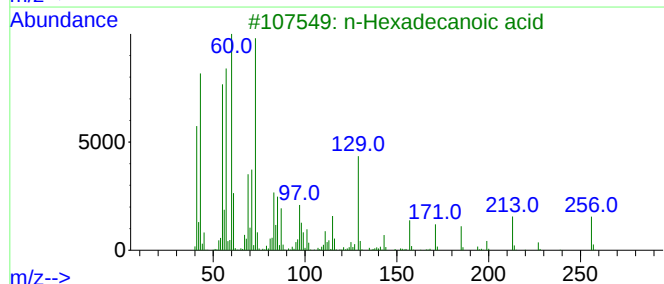
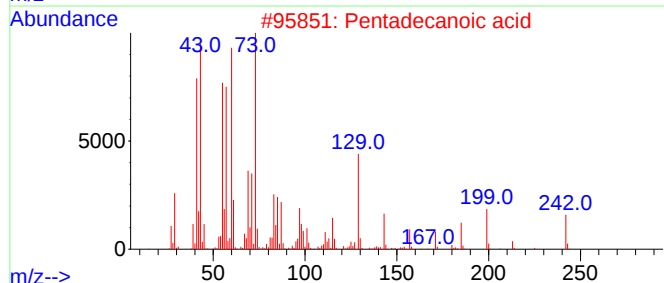
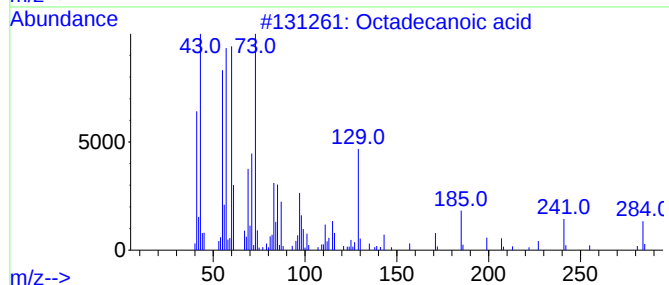
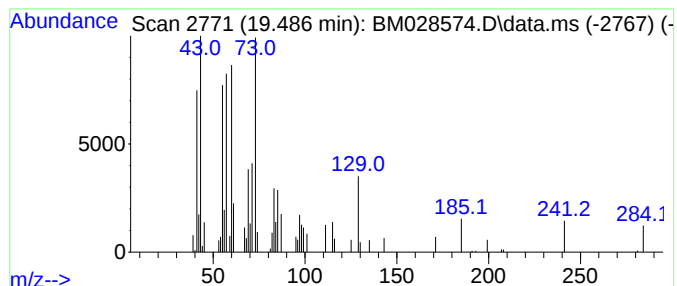
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.486	3.47 ng	48158	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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ALS Vial : 10 Sample Multiplier: 1

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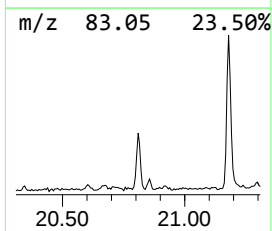
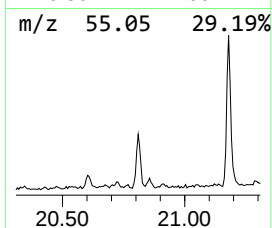
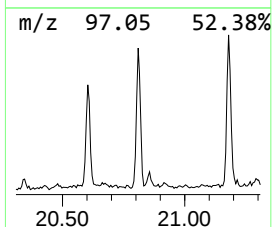
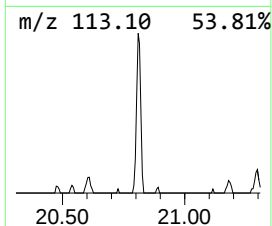
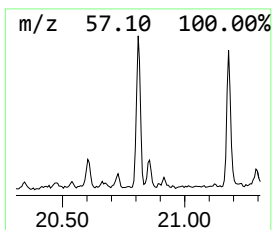
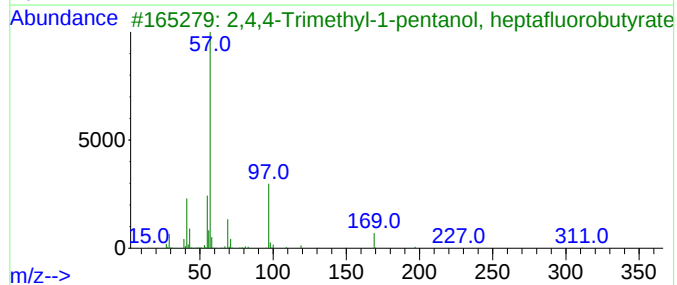
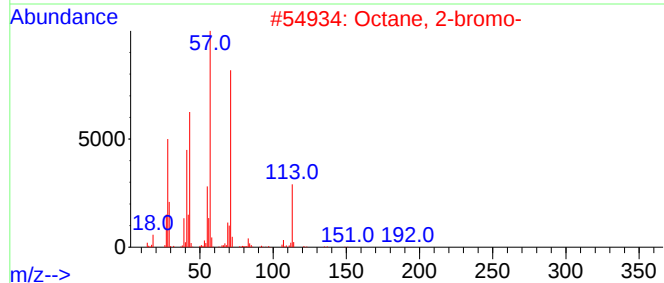
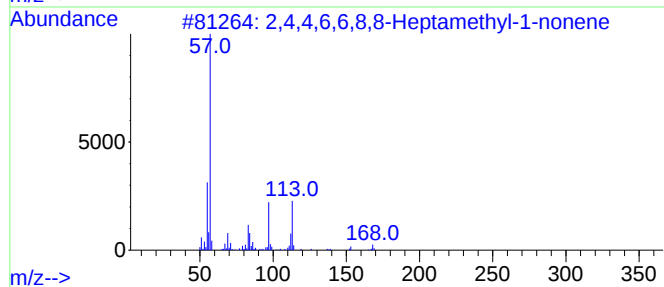
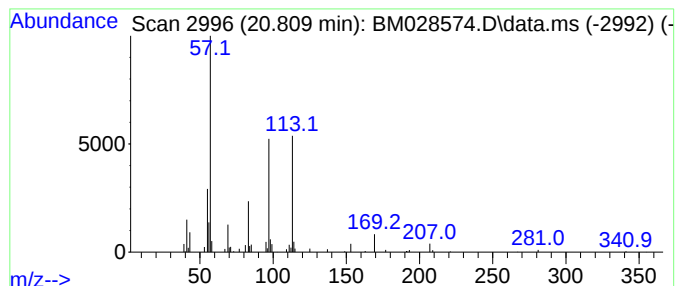
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Peak Number 4 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.809	3.91 ng	54181	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	59		
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35		
3	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	35		
4	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	25		
5	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	25		



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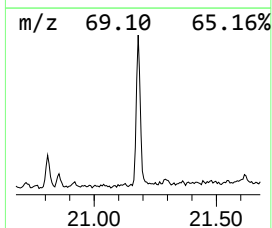
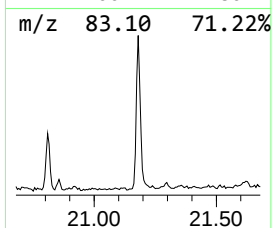
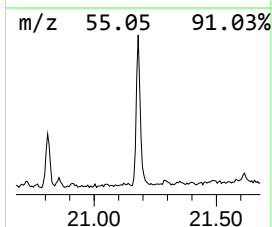
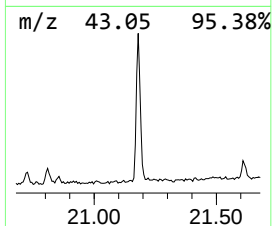
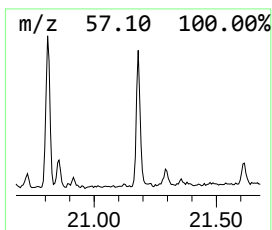
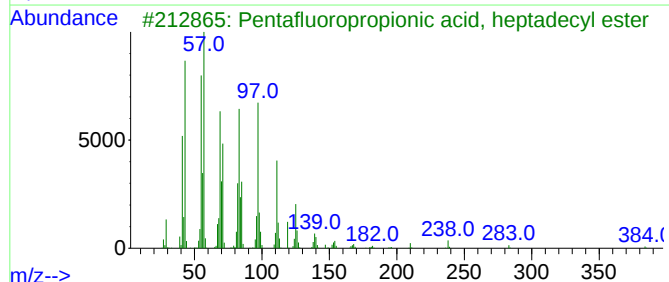
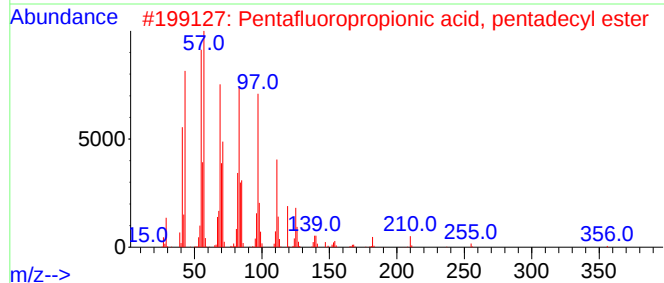
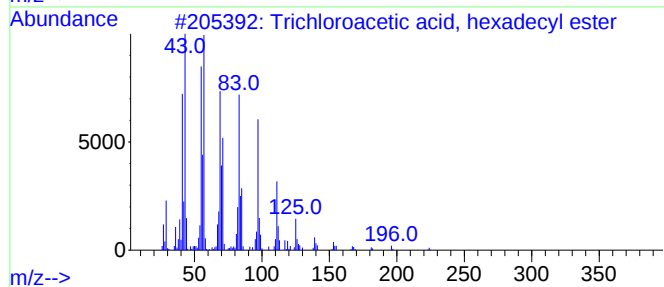
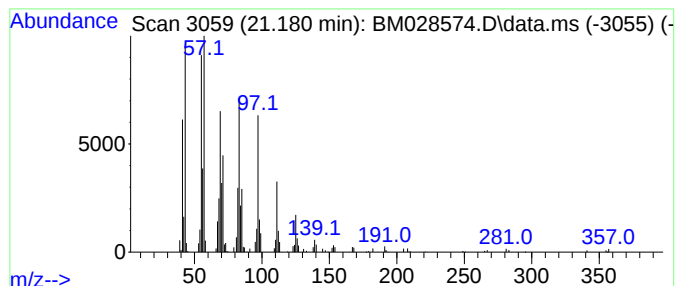
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	8.65 ng	119911	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.221	9.3	ng	110308	4	17.345	237963	20.0
unknown18.974	18.974	4.4	ng	52631	4	17.345	237963	20.0
Octadecanoic acid	19.486	3.5	ng	48158	5	21.480	277263	20.0
2,4,4,6,6,8,8-H...	20.809	3.9	ng	54181	5	21.480	277263	20.0
Trichloroacetic...	21.180	8.7	ng	119911	5	21.480	277263	20.0