

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
 Data File : BM028587.D
 Acq On : 28 Jan 2021 14:54
 Operator : CG/JU
 Sample : M1249-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 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: BM028587.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	306	312	319	rVB	8418	12762	1.33%	0.186%
2	5.516	389	396	406	rBV	461913	679030	70.88%	9.874%
3	7.157	668	675	687	rBV	454175	715048	74.63%	10.398%
4	7.963	806	812	819	rBV	116886	180036	18.79%	2.618%
5	9.140	1004	1012	1021	rBV	275469	449343	46.90%	6.534%
6	10.781	1284	1291	1299	rVB	147927	244720	25.54%	3.559%
7	13.233	1702	1708	1716	rBV	563337	819678	85.56%	11.919%
8	14.063	1843	1849	1855	rVB	11782	16684	1.74%	0.243%
9	14.251	1875	1881	1887	rBV2	6420	10058	1.05%	0.146%
10	14.610	1936	1942	1949	rBV	194876	290238	30.29%	4.220%
11	16.098	2189	2195	2208	rBV	450167	615856	64.28%	8.955%
12	17.345	2401	2407	2412	rBV	216090	304877	31.82%	4.433%
13	18.110	2531	2537	2540	rBV4	5399	9812	1.02%	0.143%
14	18.163	2543	2546	2550	rBV3	7805	11749	1.23%	0.171%
15	18.221	2551	2556	2566	rBV	143709	194170	20.27%	2.823%
16	18.504	2600	2604	2609	rBV3	6468	9670	1.01%	0.141%
17	18.710	2635	2639	2644	rVB	11064	16777	1.75%	0.244%
18	18.968	2679	2683	2688	rBV	76036	96325	10.05%	1.401%
19	19.057	2694	2698	2706	rBV	21960	30293	3.16%	0.440%
20	19.127	2706	2710	2717	rVB2	9266	14685	1.53%	0.214%
21	19.380	2749	2753	2759	rVB3	19713	35114	3.67%	0.511%
22	19.486	2767	2771	2780	rBV	77544	114388	11.94%	1.663%
23	19.604	2787	2791	2796	rVB	21008	23883	2.49%	0.347%
24	19.745	2812	2815	2821	rVB2	12137	18221	1.90%	0.265%
25	19.939	2843	2848	2854	rBV	771204	958061	100.00%	13.931%
26	20.133	2877	2881	2885	rVB	11032	14357	1.50%	0.209%
27	20.233	2896	2898	2902	rVB2	9761	10202	1.06%	0.148%
28	20.604	2958	2961	2967	rVB	22620	30821	3.22%	0.448%
29	20.809	2992	2996	3001	rBV	90022	106405	11.11%	1.547%
30	20.856	3001	3004	3008	rVB2	22225	25584	2.67%	0.372%
31	21.180	3055	3059	3064	rBV	122269	144702	15.10%	2.104%
32	21.480	3105	3110	3115	rBV2	262641	343737	35.88%	4.998%
33	23.750	3490	3496	3503	rVB2	173545	329711	34.41%	4.794%

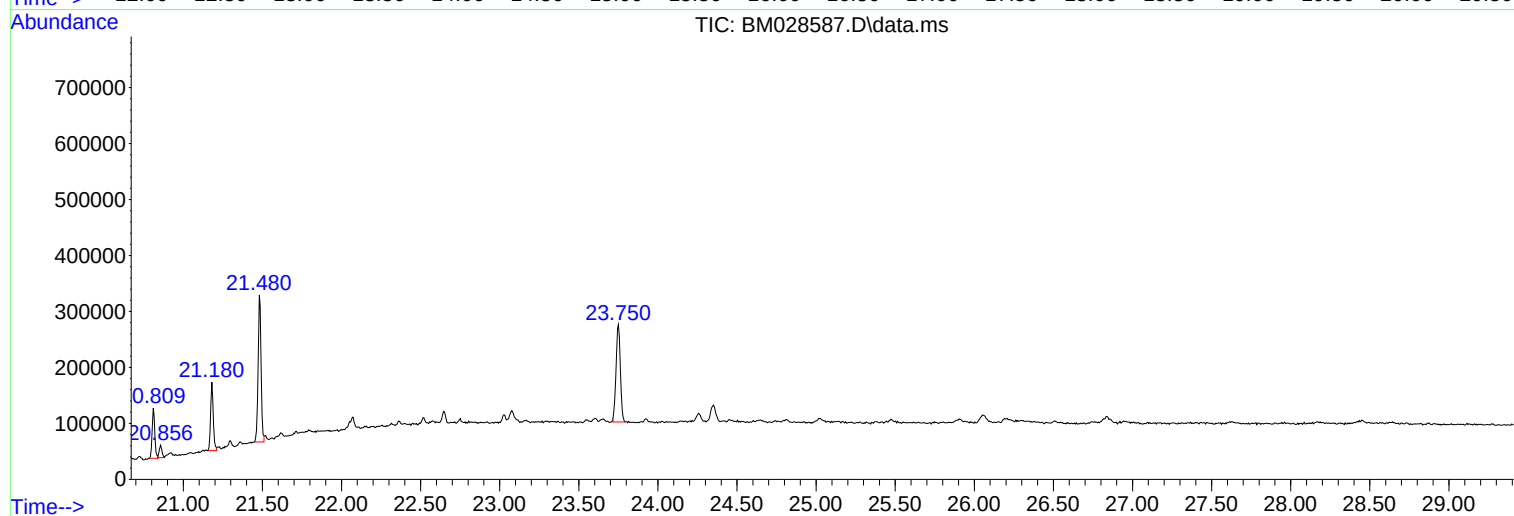
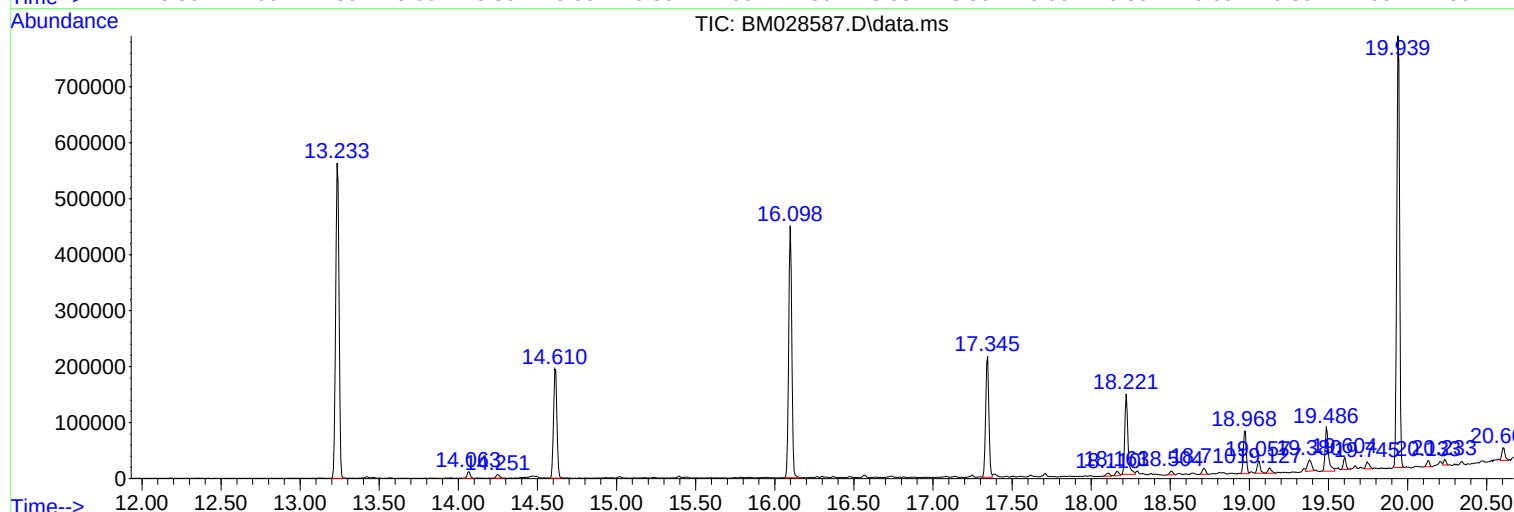
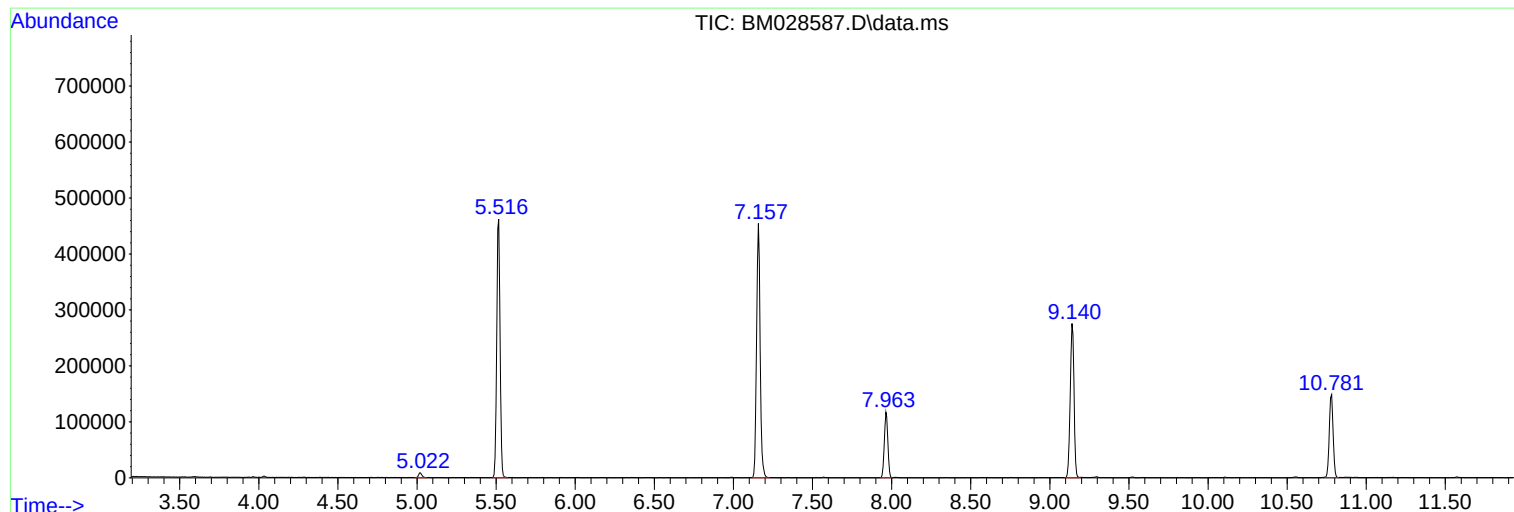
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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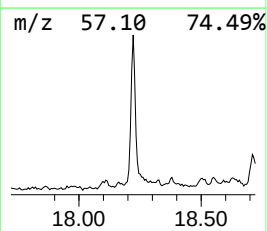
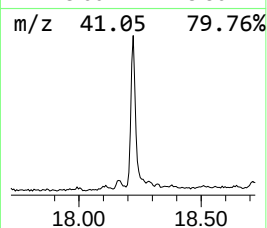
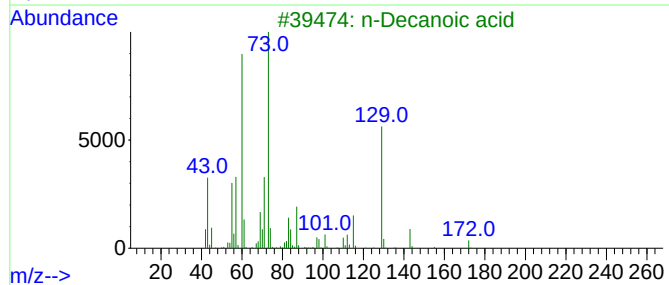
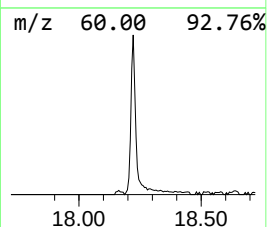
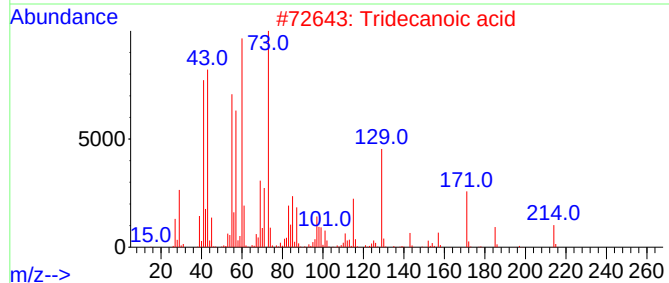
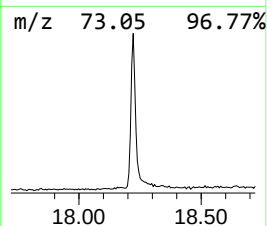
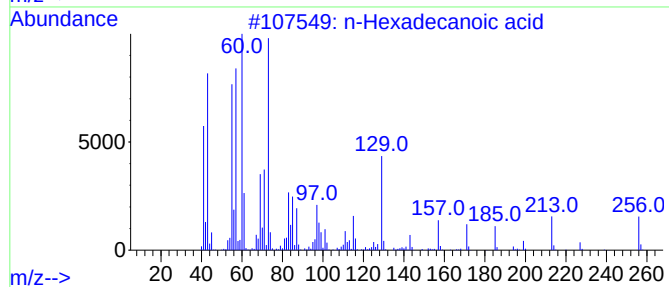
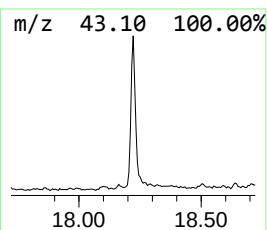
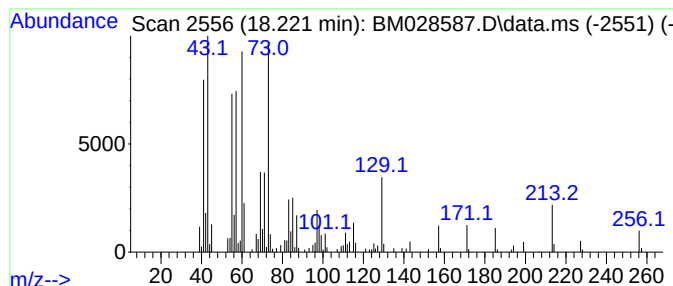
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	12.74 ng	194170	Phenanthrene-d10	17.345

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	90
3			n-Decanoic acid	172	C10H20O2	000334-48-5	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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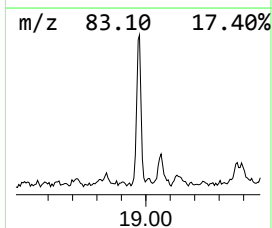
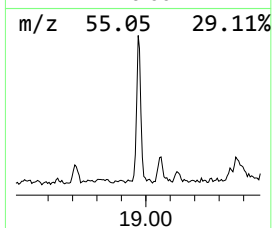
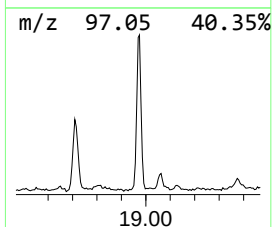
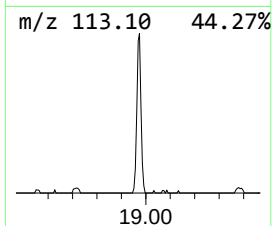
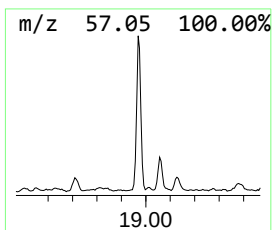
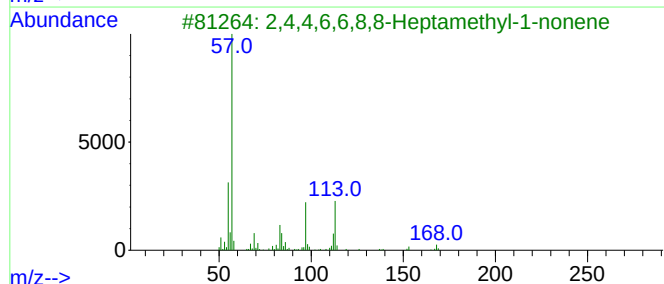
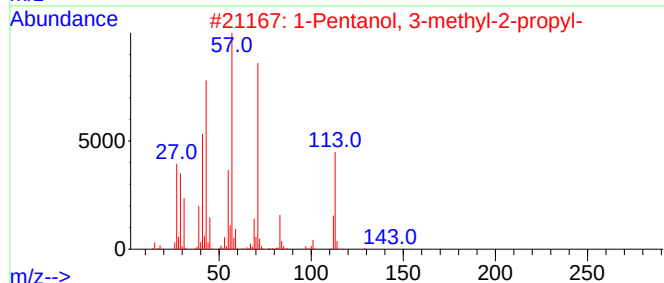
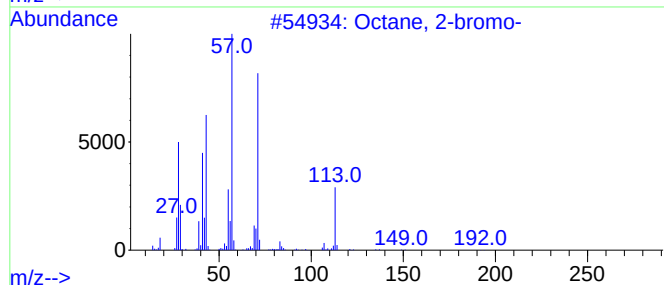
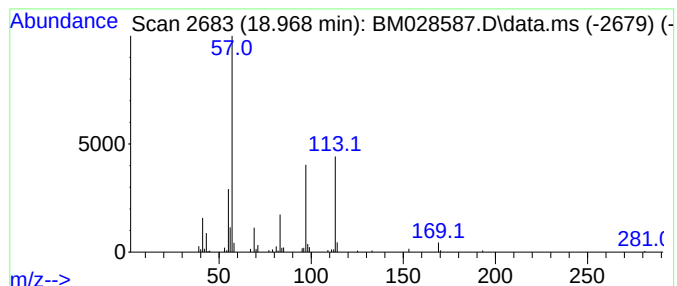
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown18.96 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.968	6.32 ng	96325	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-		192	C8H17Br		000557-35-7	47
2	1-Pentanol, 3-methyl-2-propyl-		144	C9H20O		054004-40-9	40
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene		224	C16H32		015796-04-0	38
4	2,4,4-Trimethyl-1-pentanol, hept...		326	C12H17F7O2		1000365-01-4	37
5	Formic acid, 2,4,4-trimethylpent...		158	C9H18O2		1000368-95-2	32



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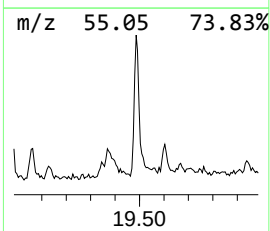
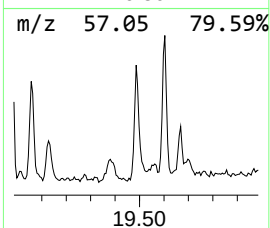
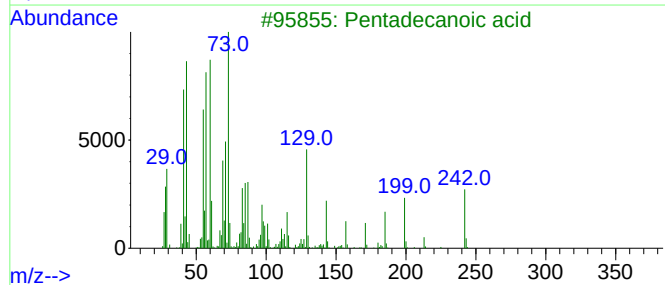
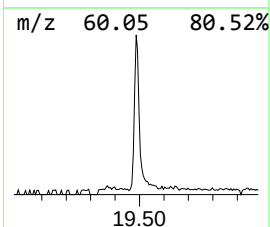
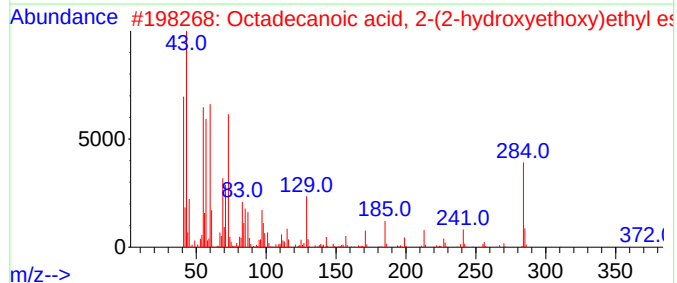
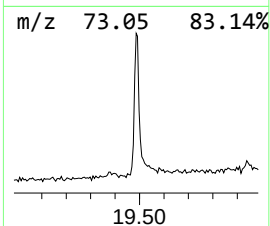
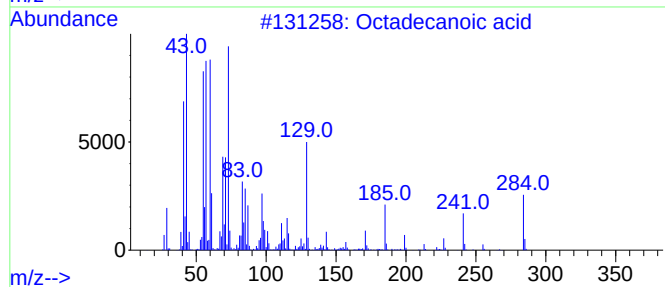
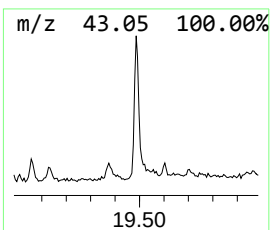
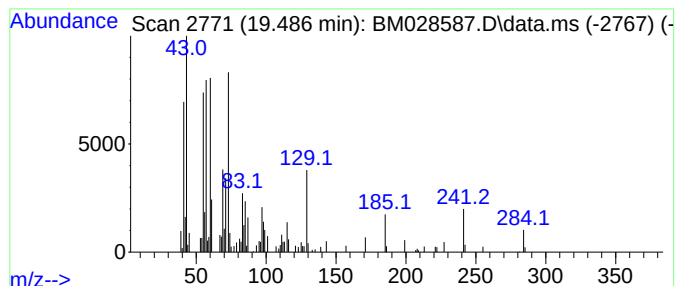
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.486	6.66 ng	114388	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	62



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampled :
1

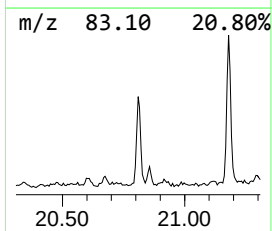
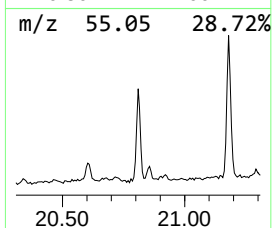
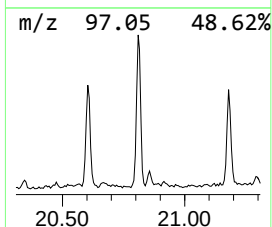
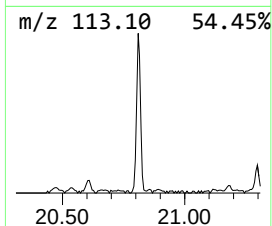
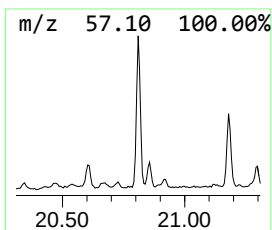
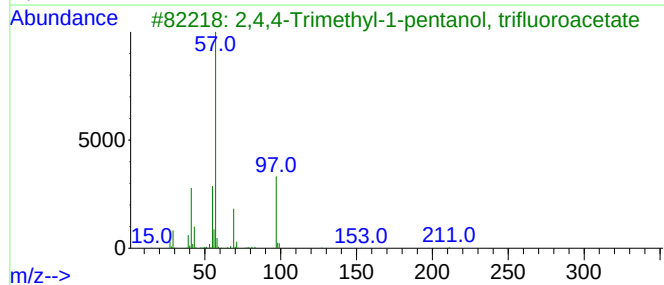
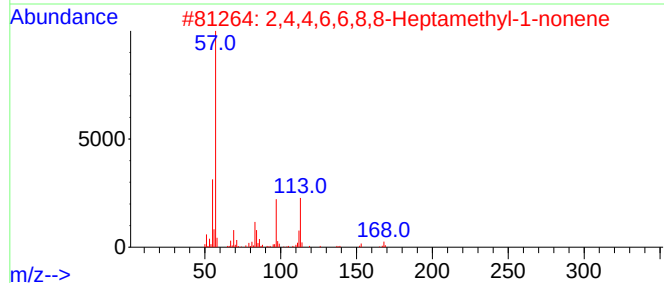
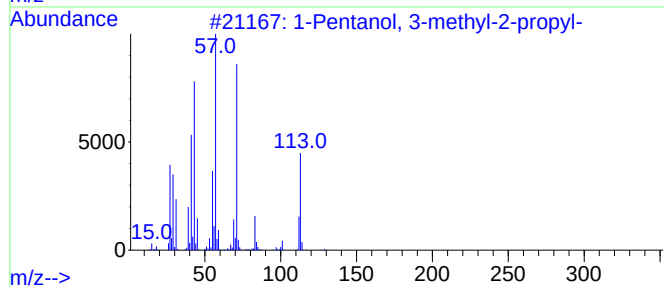
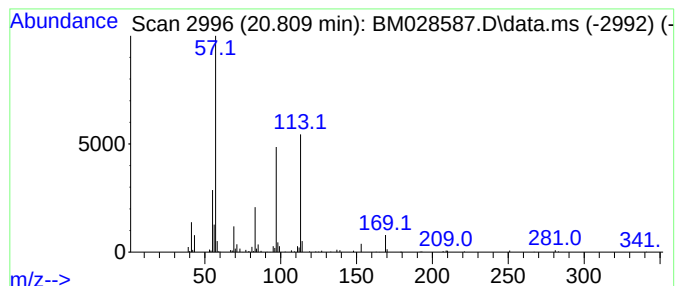
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown20.80 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.809	6.19 ng	106405	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	37
2			2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	37
3			2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	35
4			Octane, 2-bromo-	192	C8H17Br	000557-35-7	32
5			Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	25



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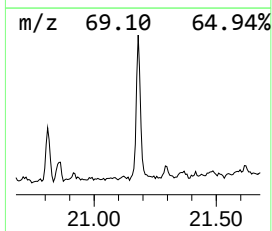
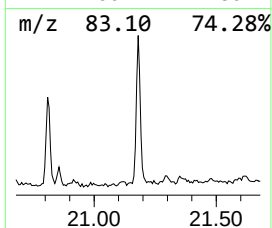
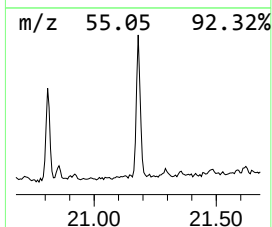
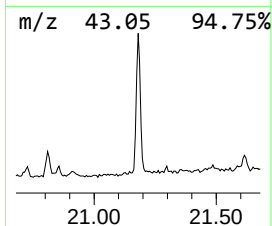
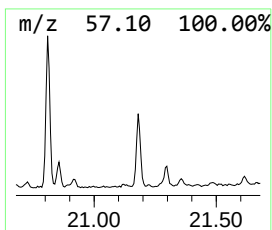
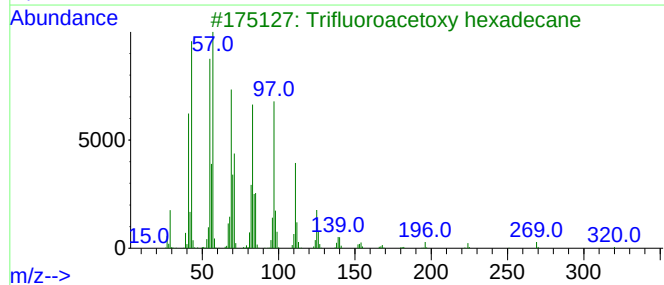
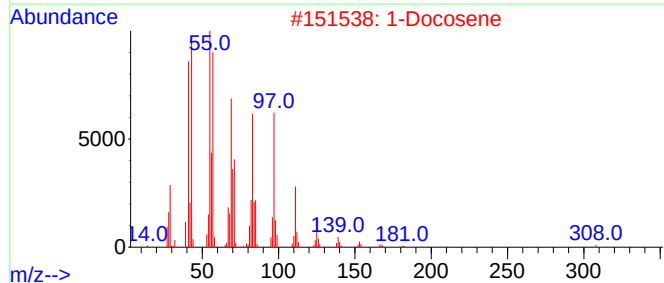
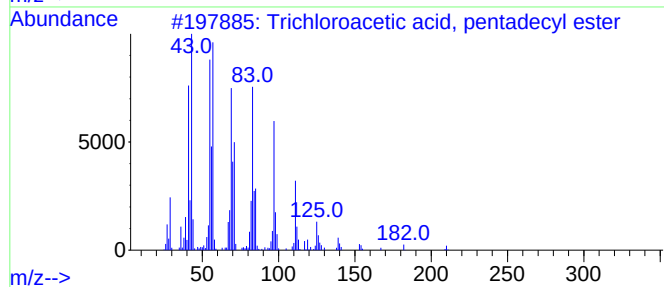
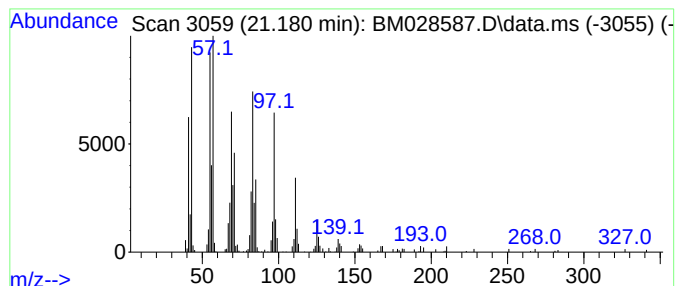
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	8.42 ng	144702	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
2			1-Docosene	308	C22H44	001599-67-3	95
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.221	12.7	ng	194170	4	17.345	304877	20.0
unknown18.96	18.968	6.3	ng	96325	4	17.345	304877	20.0
Octadecanoic acid	19.486	6.7	ng	114388	5	21.480	343737	20.0
unknown20.80	20.809	6.2	ng	106405	5	21.480	343737	20.0
Trichloroacetic...	21.180	8.4	ng	144702	5	21.480	343737	20.0