

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
 Data File : BM029716.D
 Acq On : 29 Apr 2021 19:22
 Operator : CG/JU
 Sample : M2191-01 2X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TR-05-042721

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-BM043021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029716.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.752	309	317	321	rBV3	9118	16482	1.03%	0.148%
2	5.193	386	392	405	rBV	357068	534416	33.52%	4.786%
3	6.775	653	661	677	rBV	324854	573483	35.97%	5.136%
4	7.592	793	800	812	rBV	248636	401847	25.20%	3.599%
5	8.751	990	997	1007	rBV	201824	353776	22.19%	3.168%
6	10.375	1264	1273	1287	rBV	306907	525255	32.94%	4.704%
7	12.857	1688	1695	1704	rBV	681585	1019427	63.94%	9.129%
8	13.074	1726	1732	1740	rVB3	12510	20715	1.30%	0.186%
9	13.710	1835	1840	1844	rBV	12979	20490	1.29%	0.183%
10	14.157	1910	1916	1921	rVB	13303	20234	1.27%	0.181%
11	14.245	1923	1931	1938	rBV	490717	734771	46.08%	6.580%
12	15.110	2073	2078	2083	rVB2	13757	18599	1.17%	0.167%
13	15.739	2179	2185	2195	rBV	455333	682825	42.83%	6.115%
14	15.974	2220	2225	2233	rBV3	17639	38952	2.44%	0.349%
15	16.768	2356	2360	2364	rBV3	12999	17325	1.09%	0.155%
16	16.815	2364	2368	2375	rVB5	11146	18301	1.15%	0.164%
17	16.986	2391	2397	2402	rBV	588725	857843	53.80%	7.682%
18	17.027	2402	2404	2410	rVB	46690	62733	3.93%	0.562%
19	17.121	2417	2420	2427	rVB	11420	18290	1.15%	0.164%
20	17.674	2509	2514	2518	rBV	61005	72792	4.57%	0.652%
21	17.898	2547	2552	2563	rBV2	87592	145837	9.15%	1.306%
22	18.192	2599	2602	2606	rBV4	15012	16047	1.01%	0.144%
23	18.821	2704	2709	2712	rBV	253796	319376	20.03%	2.860%
24	18.851	2712	2714	2724	rVB2	185759	244954	15.36%	2.194%
25	18.986	2734	2737	2742	rVB2	33180	37477	2.35%	0.336%
26	19.051	2743	2748	2753	rBV	81517	125903	7.90%	1.128%
27	19.186	2767	2771	2778	rBV4	49492	97012	6.08%	0.869%
28	19.409	2806	2809	2820	rVB	83445	132294	8.30%	1.185%
29	19.621	2840	2845	2853	rBV	1248054	1594454	100.00%	14.279%
30	20.903	3060	3063	3070	rBV4	101813	158178	9.92%	1.417%
31	21.174	3104	3109	3114	rBV	882642	1153706	72.36%	10.332%
32	23.350	3474	3479	3487	rVB2	609539	1132672	71.04%	10.144%

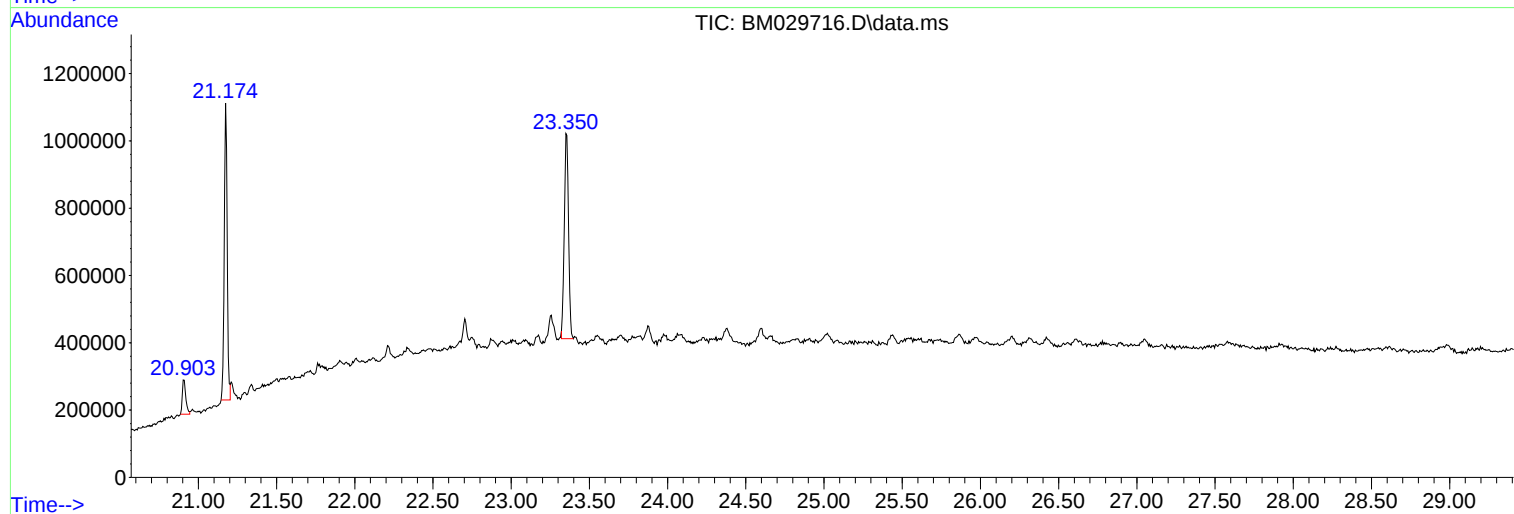
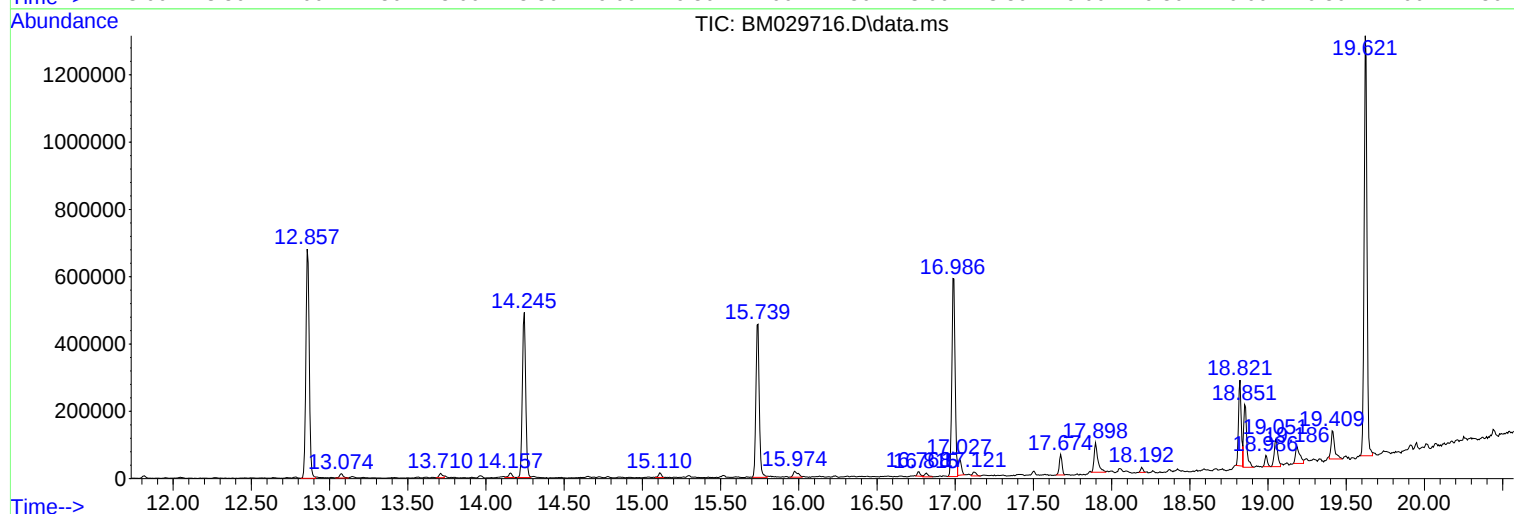
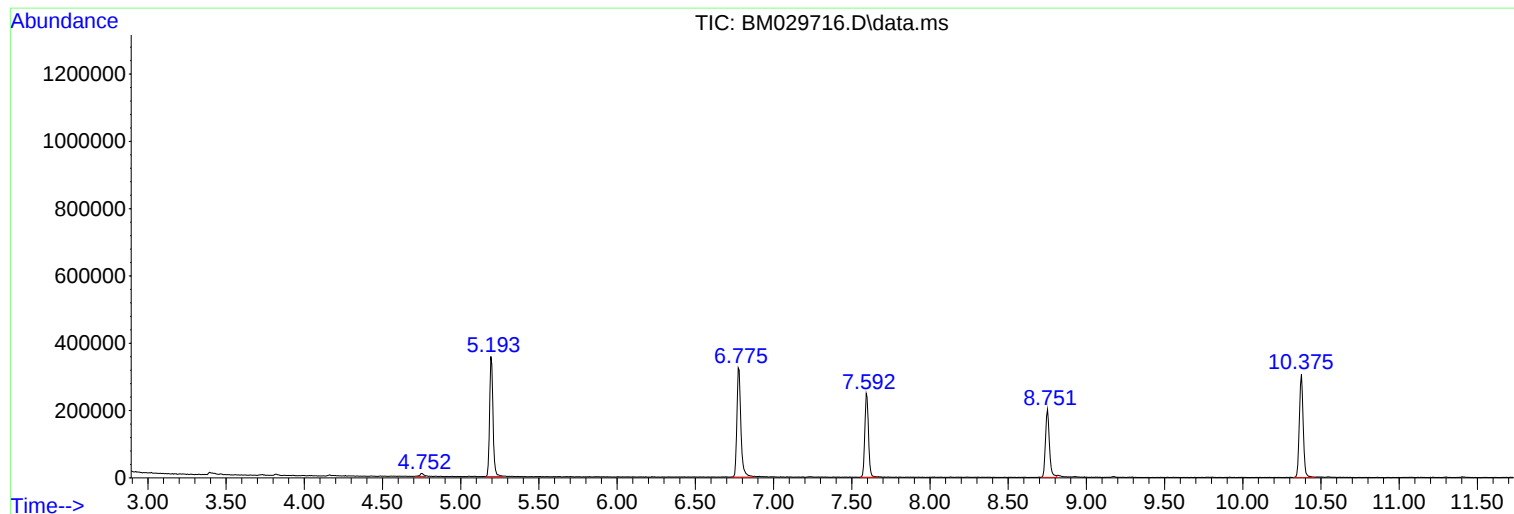
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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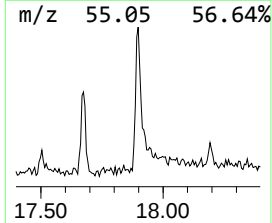
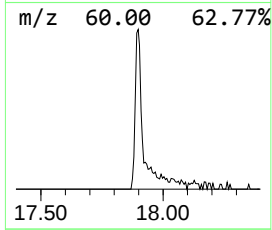
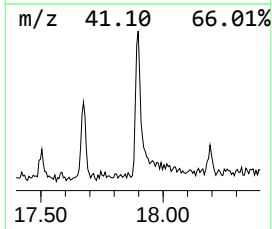
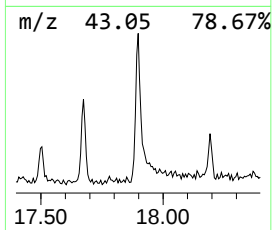
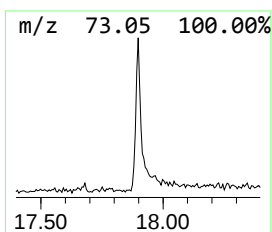
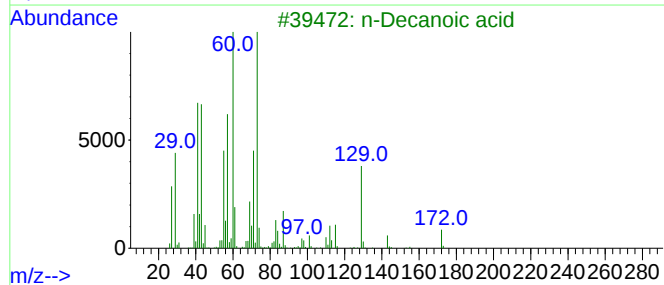
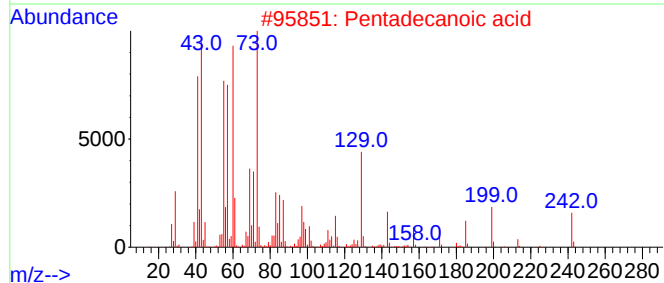
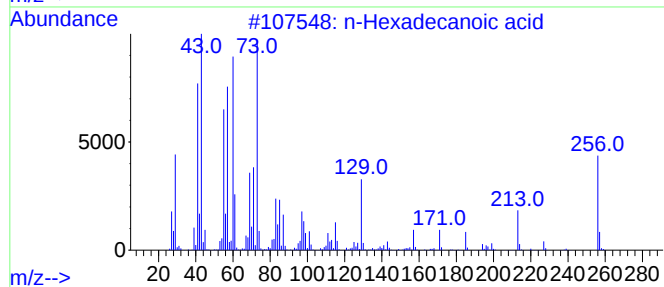
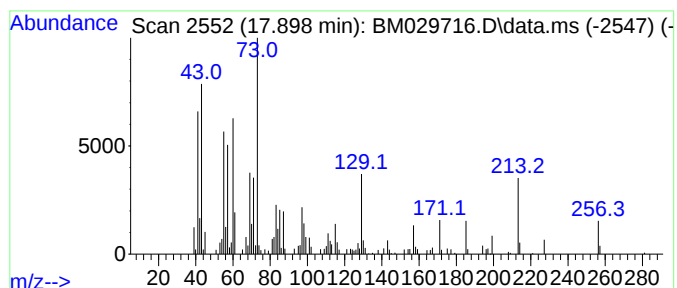
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.898	3.40 ng	145837	Phenanthrene-d10	16.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3			n-Decanoic acid	172	C10H20O2	000334-48-5	49
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	46
5			Tridecanoic acid	214	C13H26O2	000638-53-9	46



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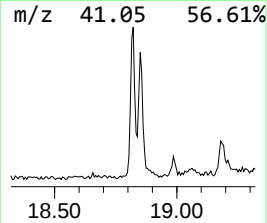
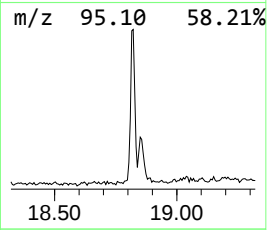
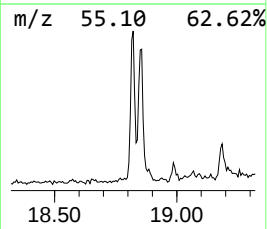
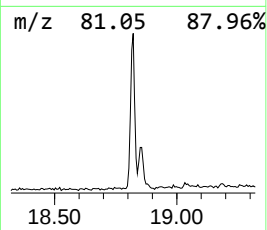
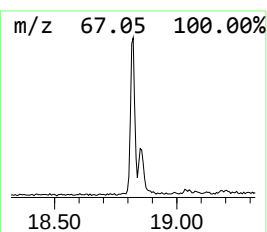
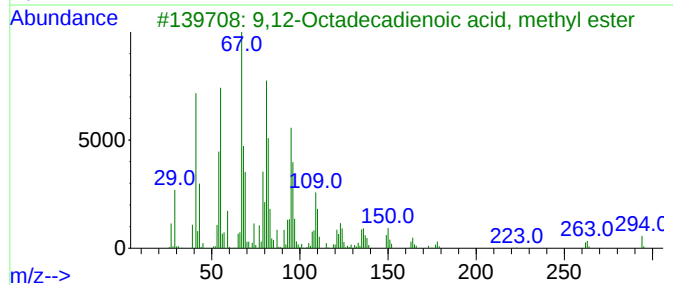
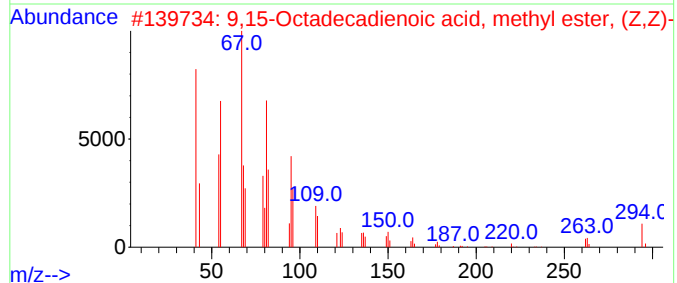
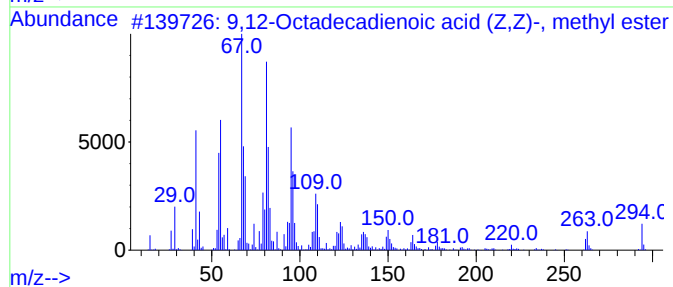
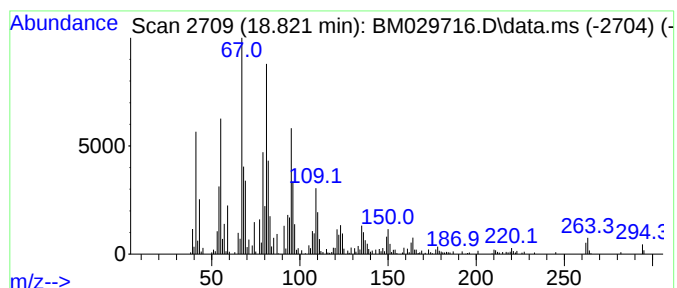
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.821	7.45 ng	319376	Phenanthrene-d10	16.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99		
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99		
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	98		
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98		
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	98		



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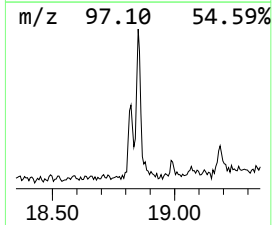
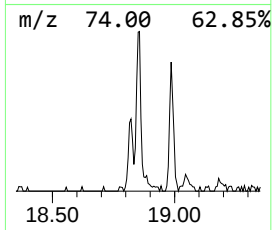
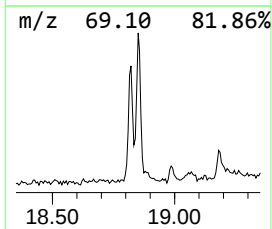
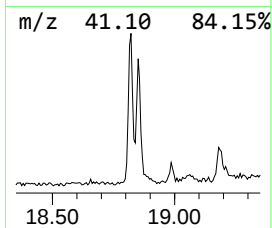
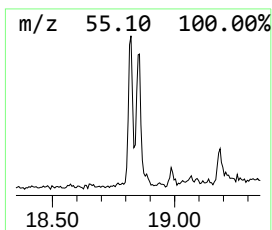
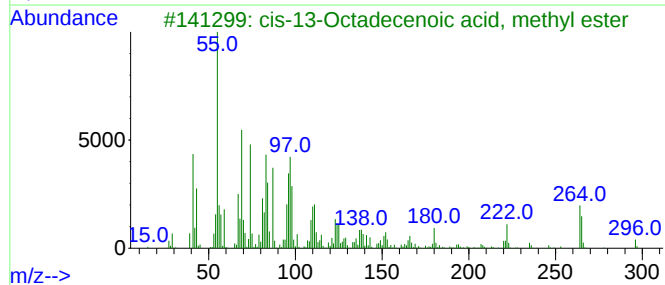
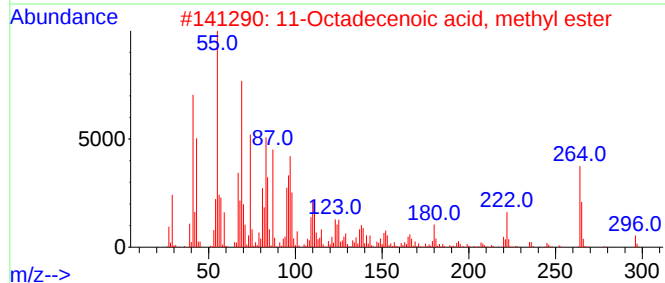
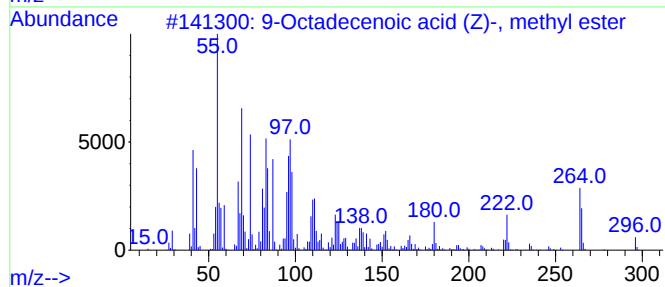
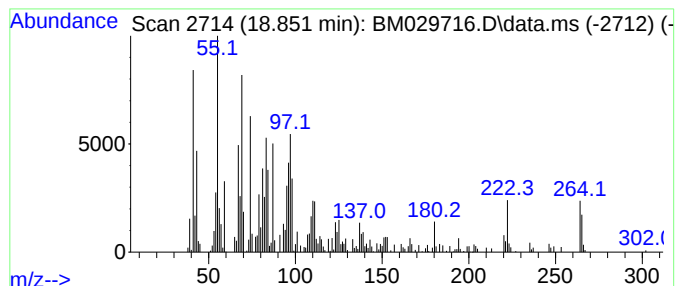
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.851	5.71 ng	244954	Phenanthrene-d10	16.992	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	87
3	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	86
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	70
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	70



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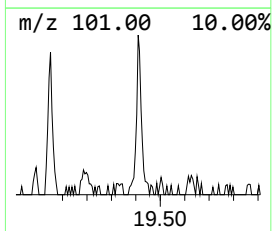
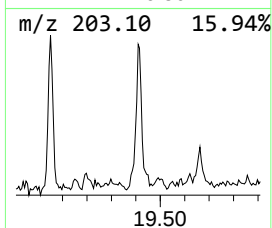
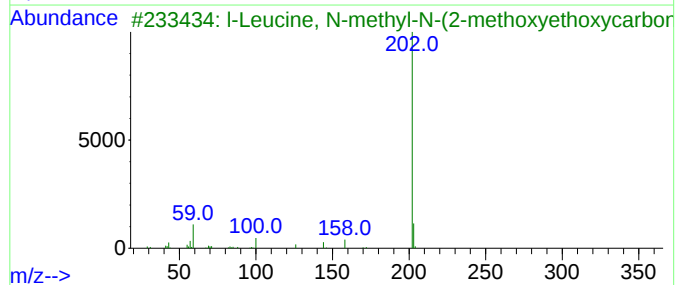
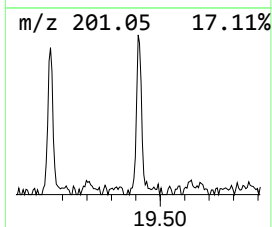
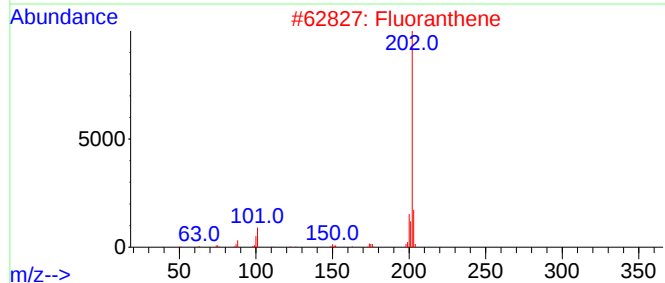
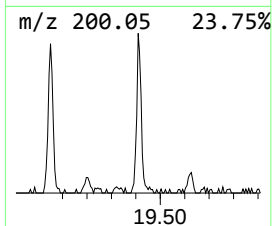
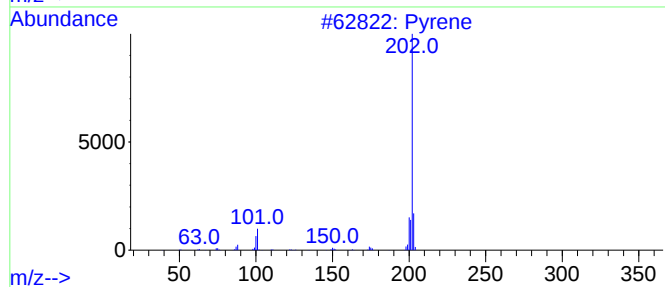
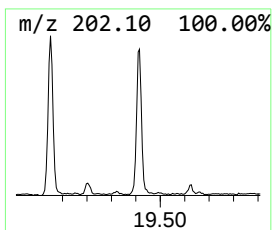
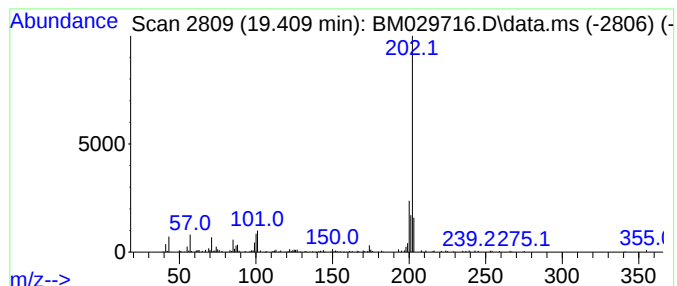
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Peak Number 5 unknown19.409 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.409	2.29 ng	132294	Chrysene-d12	21.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene	202	C16H10	000129-00-0	93
2			Fluoranthene	202	C16H10	000206-44-0	72
3			l-Leucine, N-methyl-N-(2-methoxy...	485	C28H55NO5	1000328-55-1	47
4			l-Leucyl-l-leucine, N,N'-dimethy...	430	C22H42N2O6	1000328-59-0	47
5			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	45



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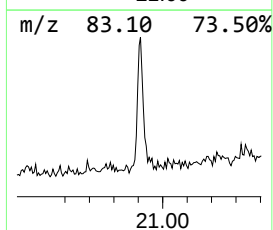
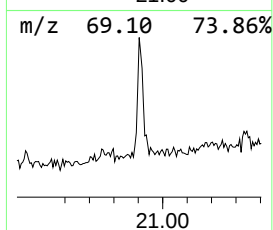
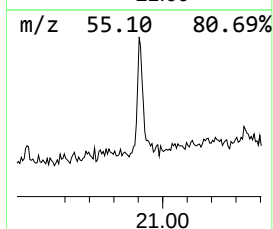
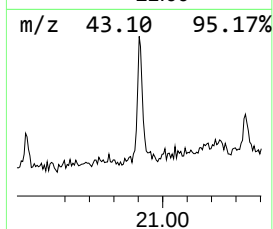
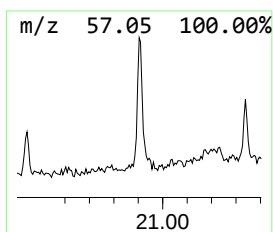
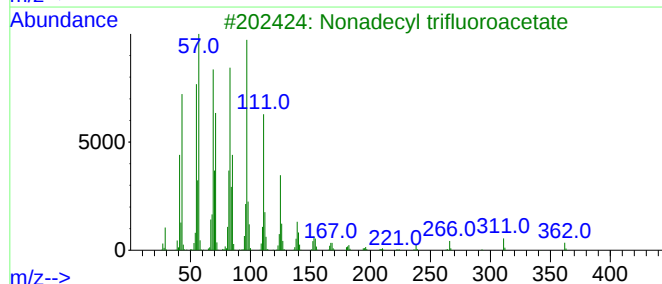
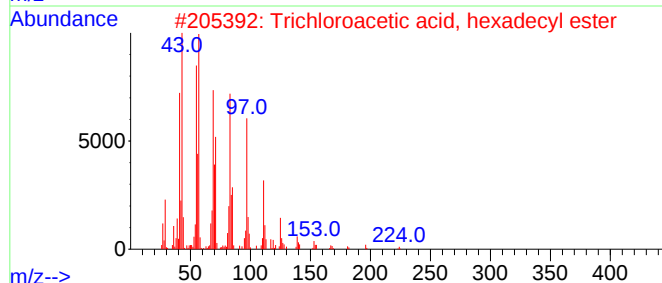
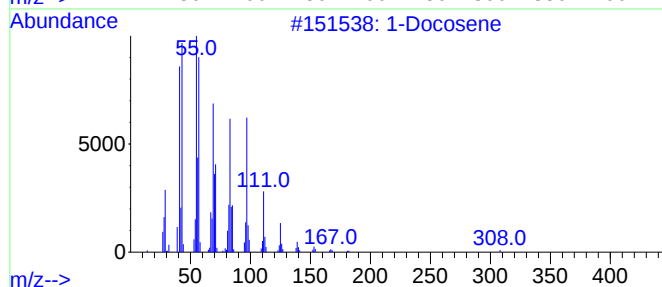
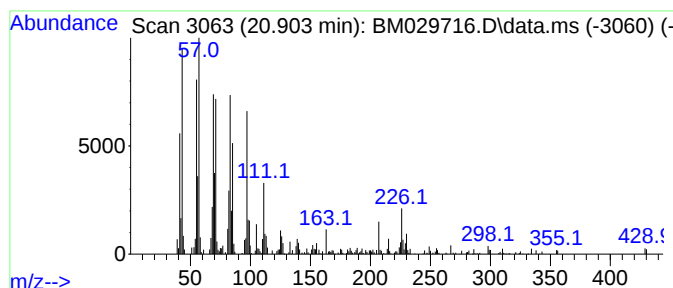
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Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.903	2.74 ng	158178	Chrysene-d12	21.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	89
2	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	83
3	Nonadecyl trifluoroacetate			380	C21H39F3O2	1000351-76-3	83
4	Trichloroacetic acid, pentadecyl...			372	C17H31Cl3O2	074339-53-0	81
5	Hexadecanoic acid, 2-hydroxy-, m...			286	C17H34O3	016742-51-1	76



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TR-05-042721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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 ...	17.898	3.4	ng	145837	4	16.992	857843	20.0
9,12-Octadecadi...	18.821	7.5	ng	319376	4	16.992	857843	20.0
9-Octadecenoic ...	18.851	5.7	ng	244954	4	16.992	857843	20.0
unknown19.409	19.409	2.3	ng	132294	5	21.174	1153710	20.0
1-Docosene	20.903	2.7	ng	158178	5	21.174	1153710	20.0