

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092321\
 Data File : BP007135.D
 Acq On : 23 Sep 2021 21:02
 Operator : CG/JU
 Sample : M3886-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 COMP-2

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_P\Methods\8270E-BP092121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007135.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.469	398	405	414	rBV	3691792	5527886	47.94%	6.723%
2	7.063	667	676	694	rBV	3512398	5703230	49.46%	6.937%
3	7.893	810	817	825	rBV	1081701	1691459	14.67%	2.057%
4	9.052	1006	1014	1027	rBV	2223827	3663466	31.77%	4.456%
5	10.475	1250	1256	1268	rBV	135610	282560	2.45%	0.344%
6	10.693	1285	1293	1299	rBV	1398894	2391962	20.74%	2.909%
7	13.145	1703	1710	1724	rBV	6158467	8924533	77.39%	10.855%
8	14.522	1936	1944	1950	rBV	2207864	3198482	27.74%	3.890%
9	14.581	1950	1954	1962	rVB	79129	128093	1.11%	0.156%
10	14.934	2006	2014	2020	rBV2	51812	124778	1.08%	0.152%
11	16.010	2190	2197	2208	rBV	4764397	7030496	60.97%	8.551%
12	17.269	2404	2411	2415	rBV	2684263	3702525	32.11%	4.503%
13	17.310	2415	2418	2424	rVV	892975	1183951	10.27%	1.440%
14	17.398	2425	2433	2438	rVB	191237	308638	2.68%	0.375%
15	17.675	2474	2480	2484	rBV2	88284	131565	1.14%	0.160%
16	18.157	2554	2562	2572	rBV2	1102883	2006709	17.40%	2.441%
17	18.322	2585	2590	2594	rBV3	182925	303755	2.63%	0.369%
18	18.616	2636	2640	2644	rBV	91153	129827	1.13%	0.158%
19	18.657	2644	2647	2652	rVB2	91346	116741	1.01%	0.142%
20	19.157	2728	2732	2736	rBV	79356	127247	1.10%	0.155%
21	19.275	2747	2752	2759	rBV	2046986	2681306	23.25%	3.261%
22	19.392	2766	2772	2783	rBV	2072821	3078363	26.70%	3.744%
23	19.598	2803	2807	2808	rBV	317284	367975	3.19%	0.448%
24	19.627	2808	2812	2820	rVB	1671900	2252443	19.53%	2.740%
25	19.827	2840	2846	2850	rBV	9424283	11531580	100.00%	14.025%
26	20.110	2891	2894	2900	rVB3	218938	335007	2.91%	0.407%
27	20.210	2908	2911	2914	rVB	128867	141899	1.23%	0.173%
28	20.839	3015	3018	3025	rVB	150724	187953	1.63%	0.229%
29	21.063	3053	3056	3063	rVB3	524657	891066	7.73%	1.084%
30	21.127	3064	3067	3072	rVV	446792	536659	4.65%	0.653%
31	21.351	3098	3105	3109	rBV2	3454638	5637870	48.89%	6.857%
32	21.386	3109	3111	3120	rVB	933327	1128596	9.79%	1.373%
33	23.021	3385	3389	3395	rBV	740984	1662830	14.42%	2.022%
34	23.651	3492	3496	3505	rVB	683944	1296808	11.25%	1.577%
35	23.763	3509	3515	3521	rVB2	1878371	3811314	33.05%	4.636%

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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_P\Methods\8270E-BP092121.M
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Sum of corrected areas: 82219572

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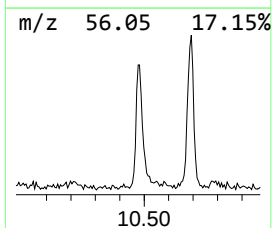
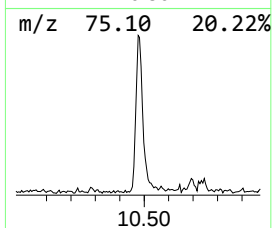
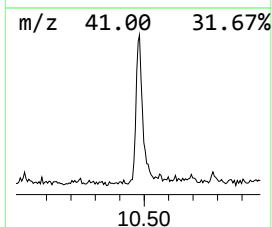
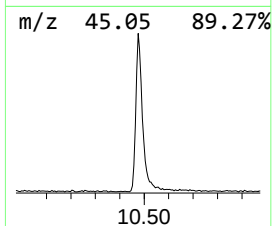
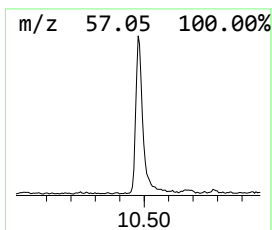
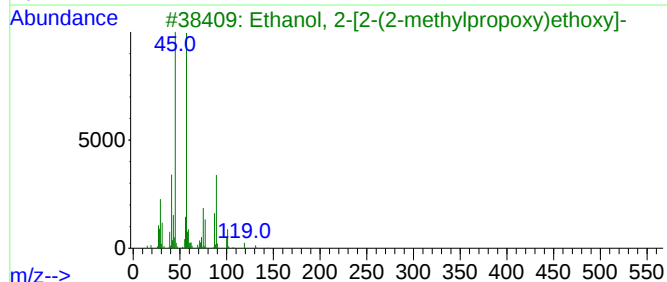
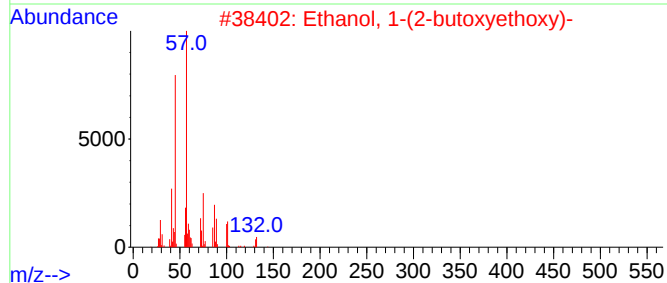
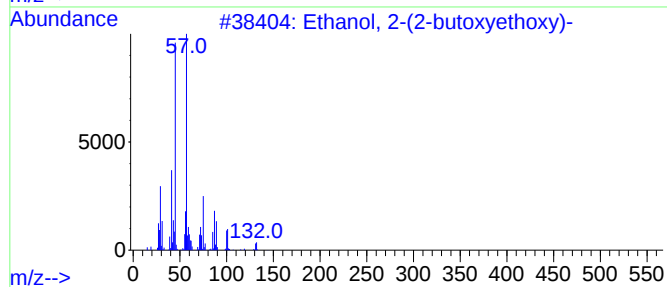
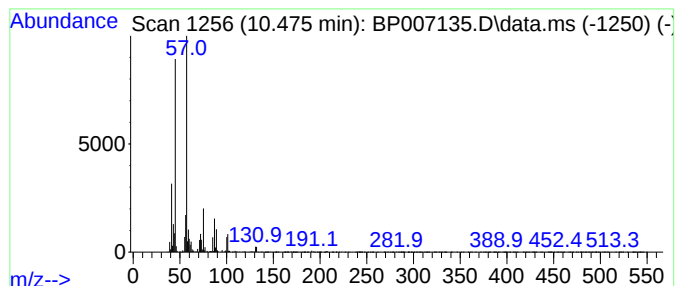
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	2.36 ng	282560	Naphthalene-d8	10.693

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			(S)-Methyl 2,3-dihydroxypropanoa...	134	C5H10O4	354578-58-8	52



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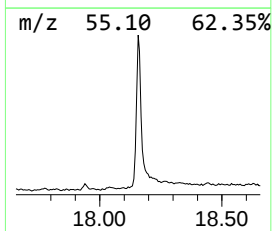
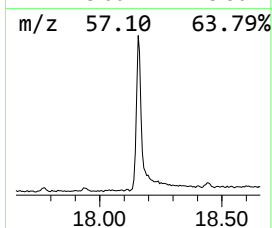
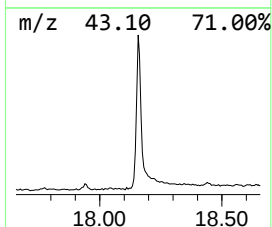
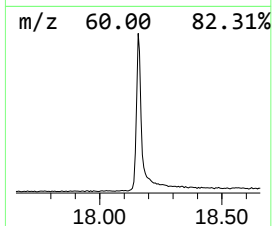
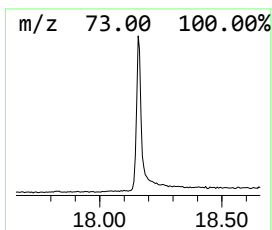
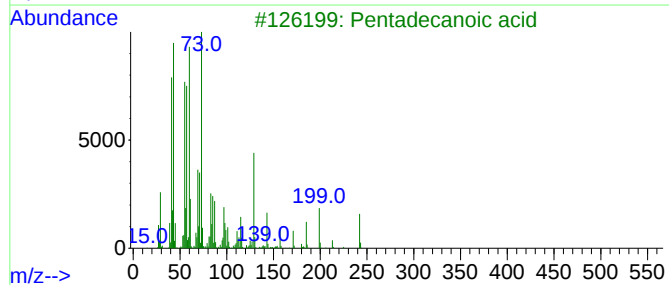
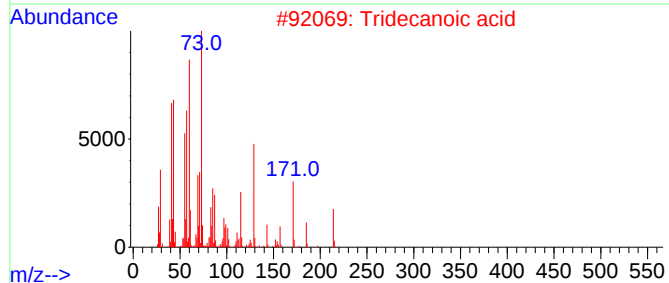
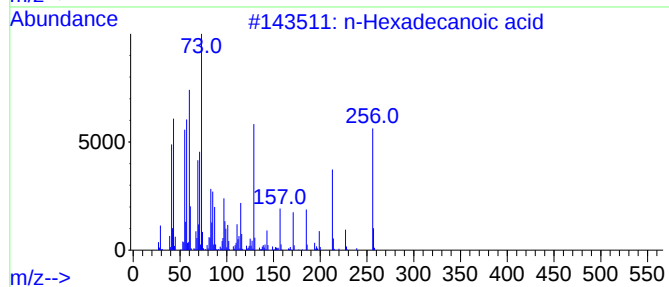
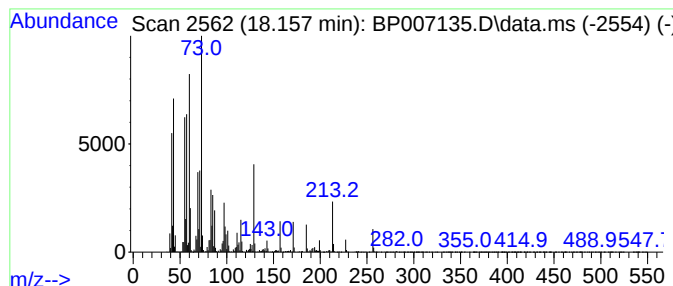
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	10.84 ng	2006710	Phenanthrene-d10	17.269

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	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5		n-Decanoic acid	172	C10H20O2	000334-48-5	58



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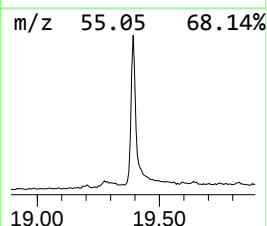
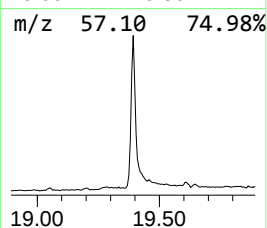
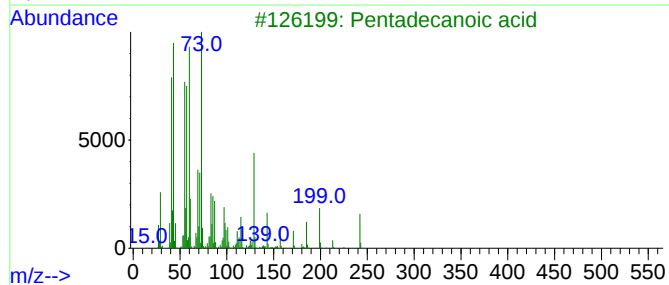
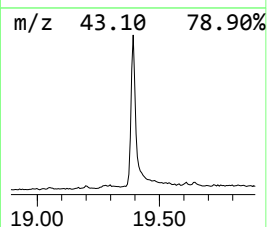
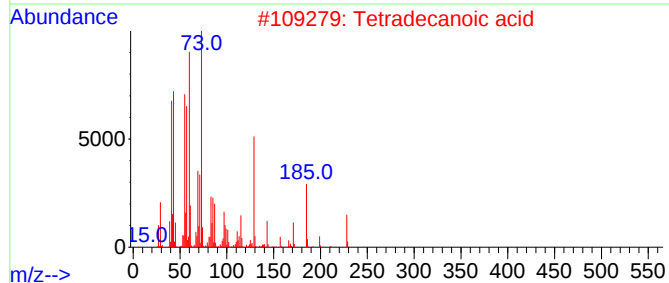
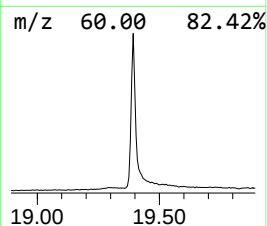
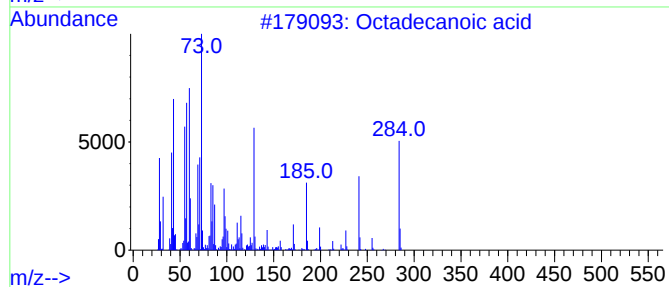
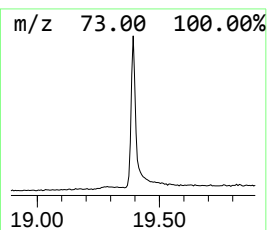
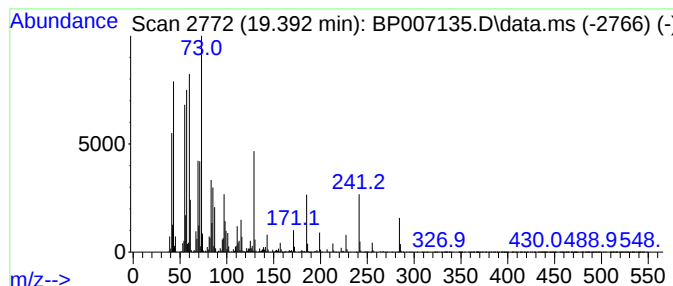
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.392	10.92 ng	3078360	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



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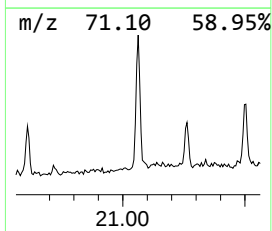
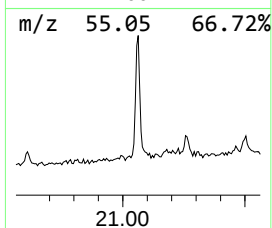
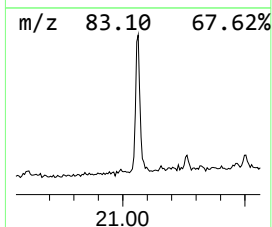
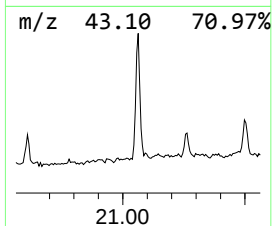
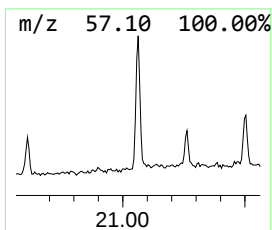
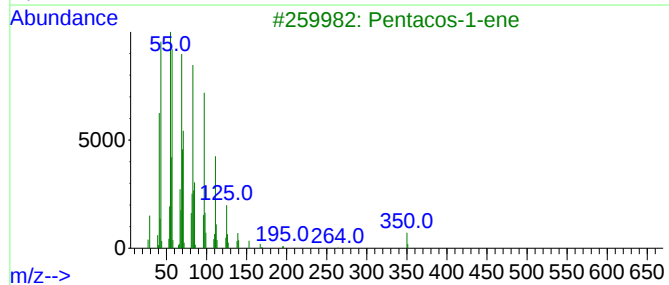
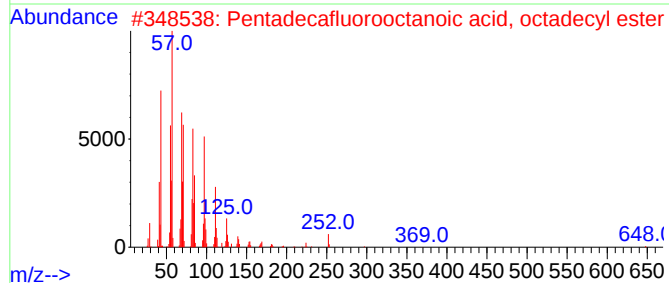
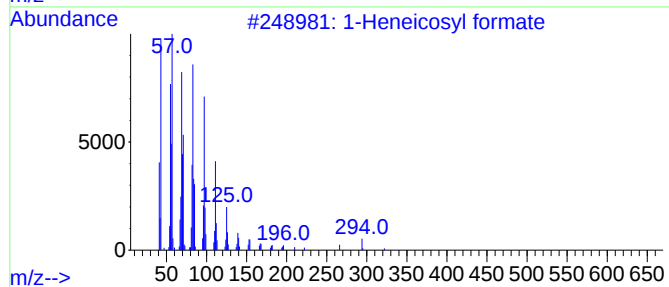
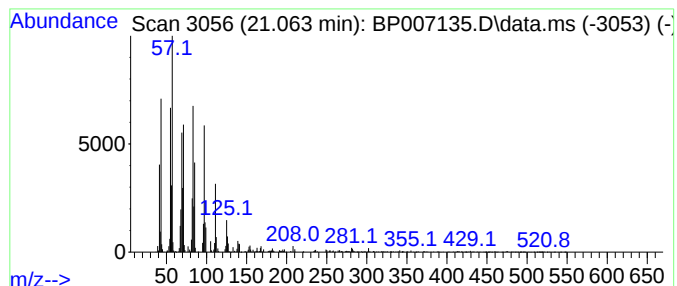
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosyl formate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	3.16 ng	891066	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	93
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	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
Ethanol, 2-(2-b...	10.475	2.4	ng	282560	2	10.693	2391960	20.0
n-Hexadecanoic ...	18.157	10.8	ng	2006710	4	17.269	3702530	20.0
Octadecanoic acid	19.392	10.9	ng	3078360	5	21.351	5637870	20.0
1-Heneicosyl fo...	21.063	3.2	ng	891066	5	21.351	5637870	20.0