

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
 Data File : BM028595.D
 Acq On : 28 Jan 2021 19:46
 Operator : CG/JU
 Sample : M1255-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 CRT-3

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: BM028595.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	307	311	319	rVB	11052	15986	1.68%	0.221%
2	5.510	388	395	405	rBV	487625	701720	73.72%	9.686%
3	7.152	667	674	685	rBV	451544	721764	75.83%	9.963%
4	7.963	804	812	819	rBV	128209	195467	20.53%	2.698%
5	9.140	1003	1012	1019	rBV	283496	454127	47.71%	6.269%
6	10.775	1284	1290	1297	rBV	158047	262682	27.60%	3.626%
7	13.233	1701	1708	1714	rBV	616077	859831	90.33%	11.869%
8	14.063	1843	1849	1855	rBV	9359	13932	1.46%	0.192%
9	14.245	1875	1880	1891	rVB2	7790	12723	1.34%	0.176%
10	14.492	1919	1922	1928	rVB2	8538	11104	1.17%	0.153%
11	14.610	1936	1942	1952	rVB2	215981	312688	32.85%	4.316%
12	15.439	2078	2083	2088	rVB2	8327	11174	1.17%	0.154%
13	16.098	2189	2195	2208	rVB	440227	614378	64.54%	8.481%
14	16.298	2225	2229	2238	rVB3	7864	12497	1.31%	0.173%
15	17.086	2356	2363	2367	rBV4	7344	11608	1.22%	0.160%
16	17.339	2401	2406	2411	rBV	235164	328355	34.50%	4.532%
17	17.386	2411	2414	2420	rVB2	8952	13152	1.38%	0.182%
18	17.710	2462	2469	2474	rBV	9125	14396	1.51%	0.199%
19	18.110	2530	2537	2542	rBV2	5625	10562	1.11%	0.146%
20	18.221	2550	2556	2565	rBV	125803	179501	18.86%	2.478%
21	18.710	2634	2639	2644	rBV	13176	21439	2.25%	0.296%
22	18.968	2678	2683	2688	rBV	91333	112618	11.83%	1.555%
23	19.057	2694	2698	2705	rBV	25086	32664	3.43%	0.451%
24	19.127	2705	2710	2716	rVV3	10519	16106	1.69%	0.222%
25	19.380	2749	2753	2759	rVB	28905	41894	4.40%	0.578%
26	19.486	2767	2771	2779	rBV	68434	92697	9.74%	1.280%
27	19.598	2787	2790	2796	rVB	22672	28299	2.97%	0.391%
28	19.745	2811	2815	2821	rVB2	19794	31834	3.34%	0.439%
29	19.939	2843	2848	2853	rBV	803221	951873	100.00%	13.139%
30	20.127	2877	2880	2884	rVB	15299	17911	1.88%	0.247%
31	20.604	2958	2961	2967	rVB	32828	43245	4.54%	0.597%
32	20.809	2992	2996	3000	rBV	116332	130405	13.70%	1.800%
33	20.857	3001	3004	3007	rVB	23587	24884	2.61%	0.343%
34	21.180	3055	3059	3064	rBV	139418	162587	17.08%	2.244%
35	21.380	3091	3093	3097	rVB	24308	25686	2.70%	0.355%
36	21.480	3105	3110	3115	rBV	300831	382375	40.17%	5.278%

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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_M\Methods\8270-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.745	3490	3495	3505	rVB2	196727	370422	38.92%	5.113%
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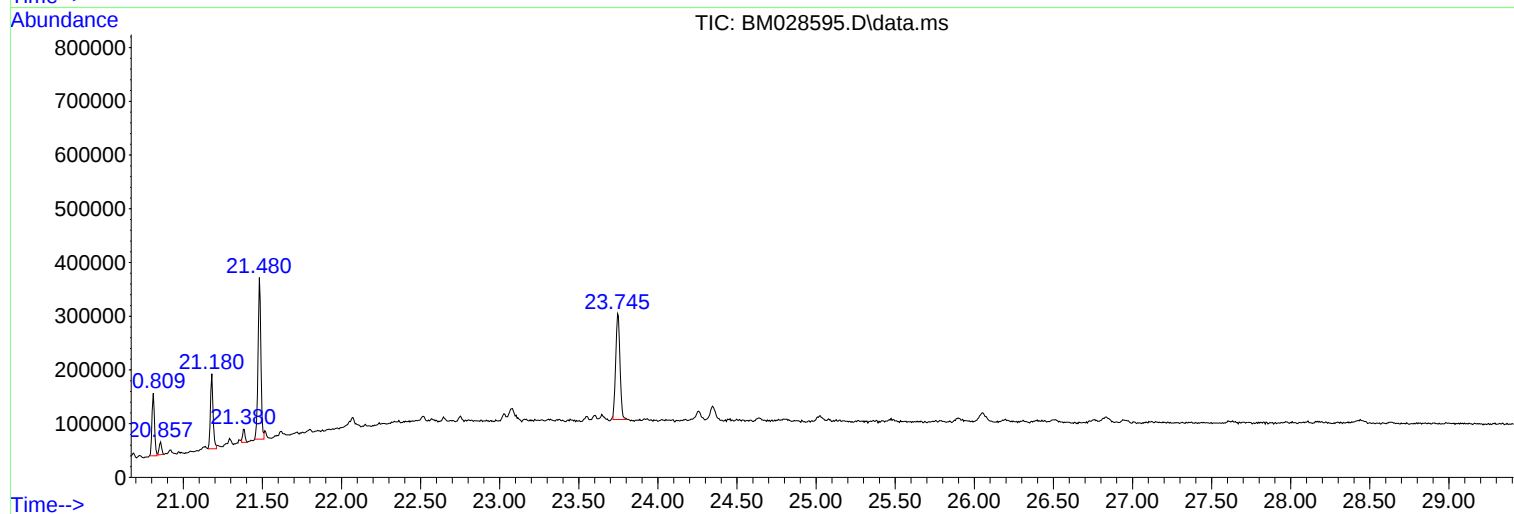
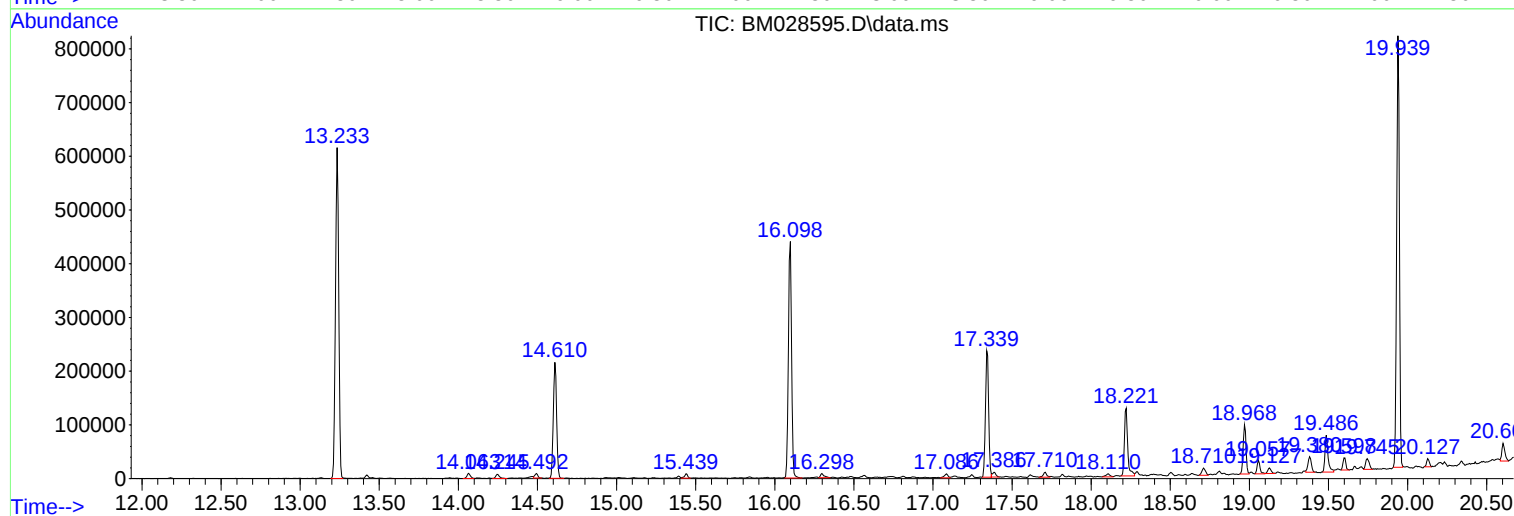
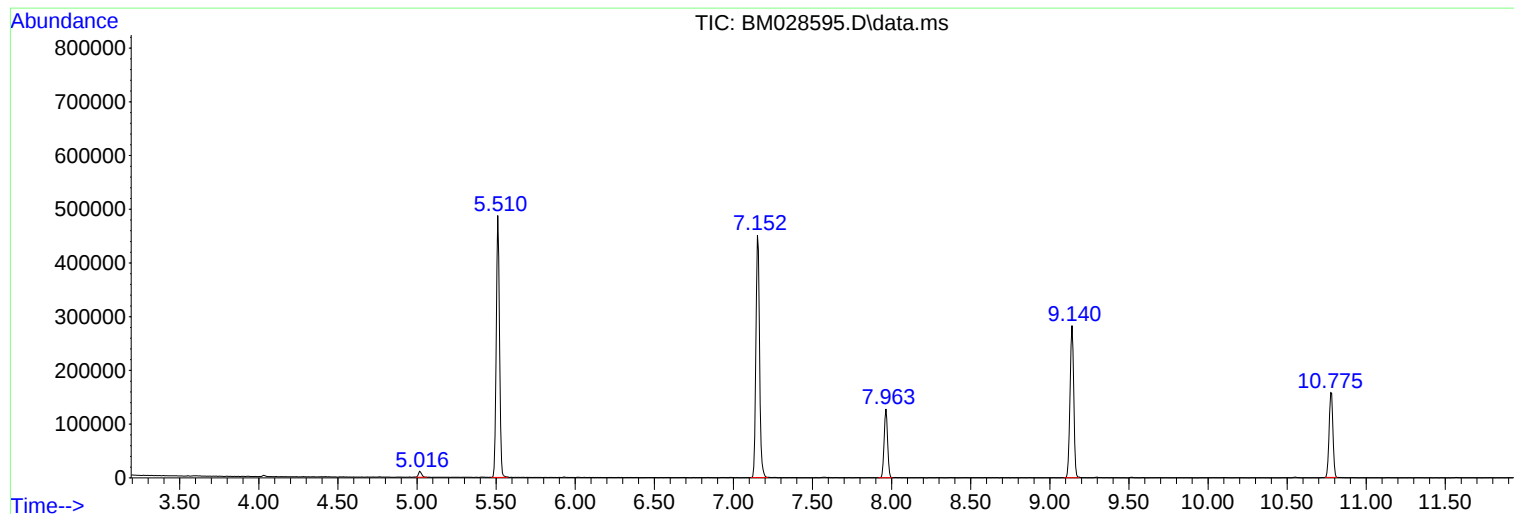
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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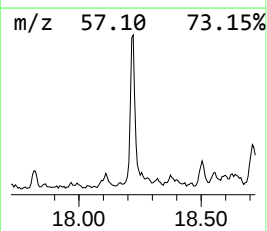
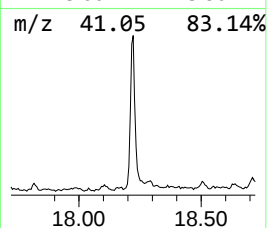
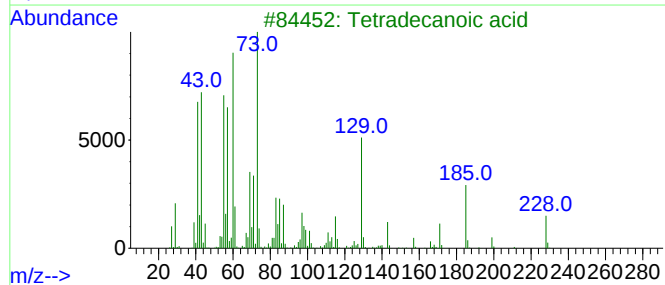
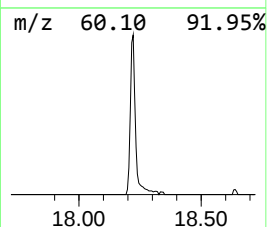
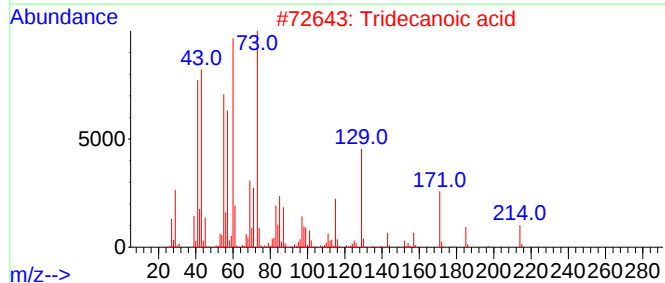
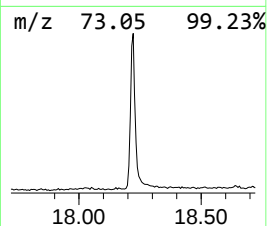
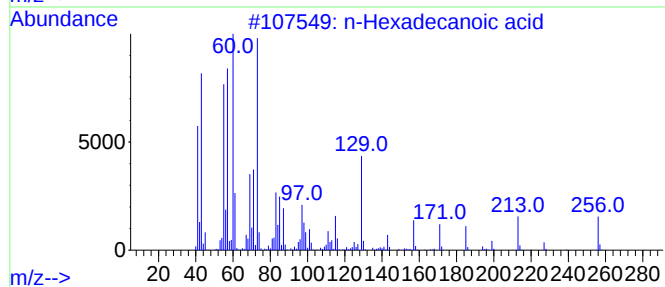
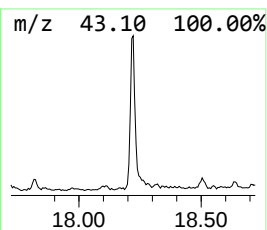
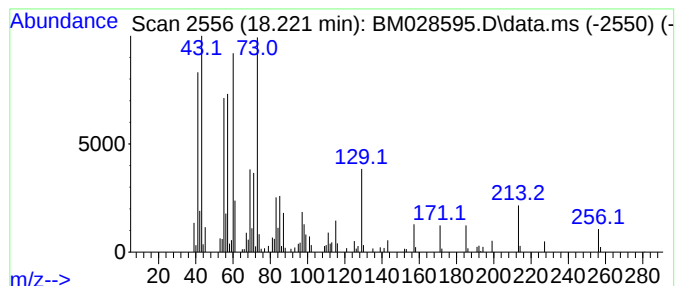
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	10.93 ng	179501	Phenanthrene-d10	17.339

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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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Instrument :
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ClientSampleId :
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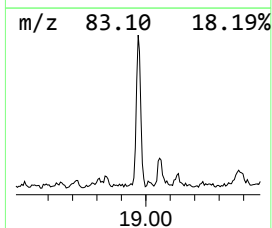
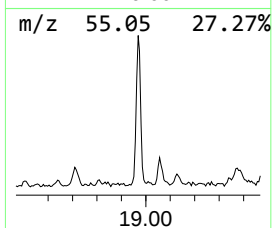
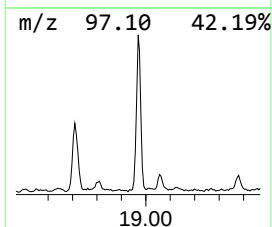
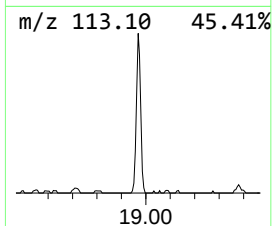
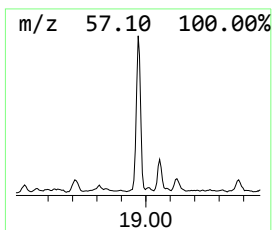
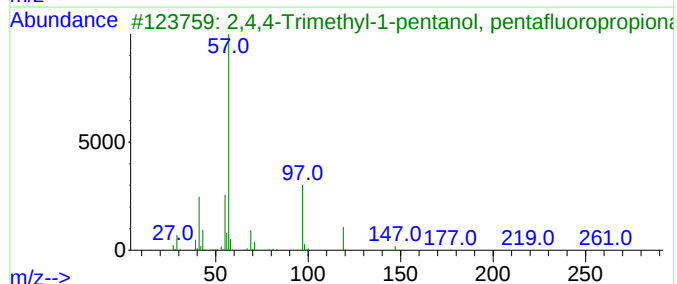
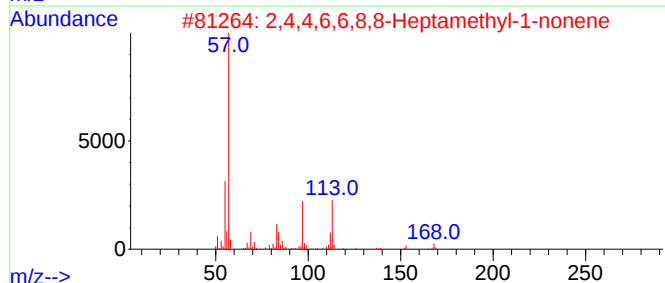
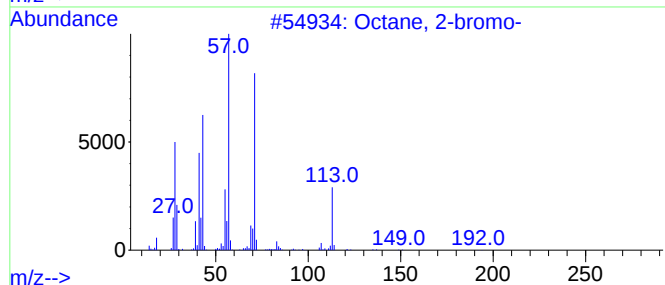
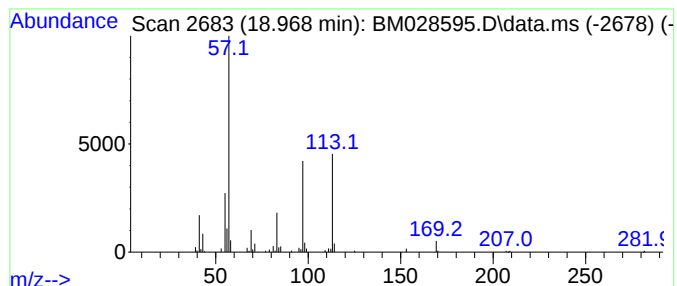
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown18.968 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.968	6.86 ng	112618	Phenanthrene-d10	17.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-		192	C8H17Br		000557-35-7	47
2	2,4,4,6,6,8,8-Heptamethyl-1-nonene		224	C16H32		015796-04-0	38
3	2,4,4-Trimethyl-1-pentanol, pent...		276	C11H17F5O2		1000365-51-0	35
4	2,4,4-Trimethyl-1-pentanol, trif...		226	C10H17F3O2		1000365-19-5	32
5	4,4-Dimethyl-3-oxopentanenitrile		125	C7H11NO		059997-51-2	32



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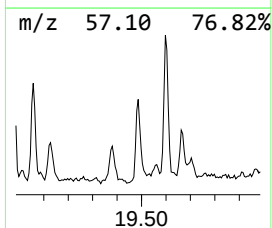
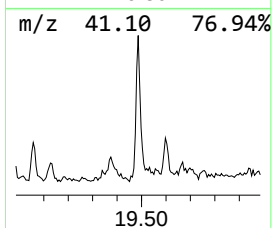
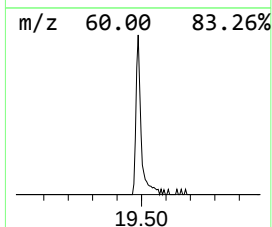
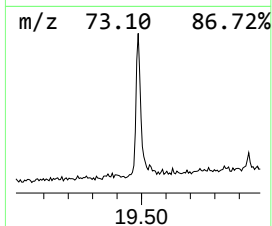
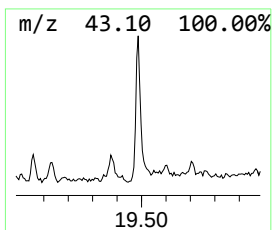
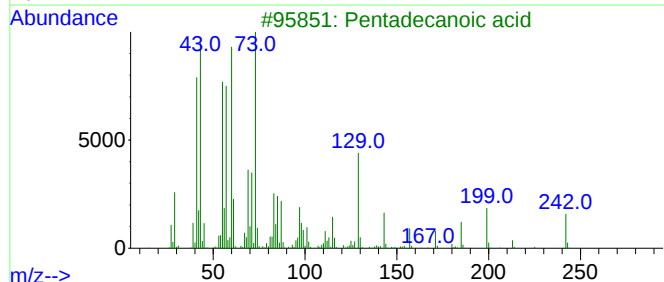
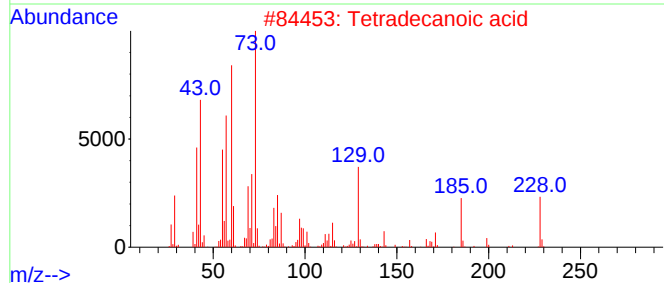
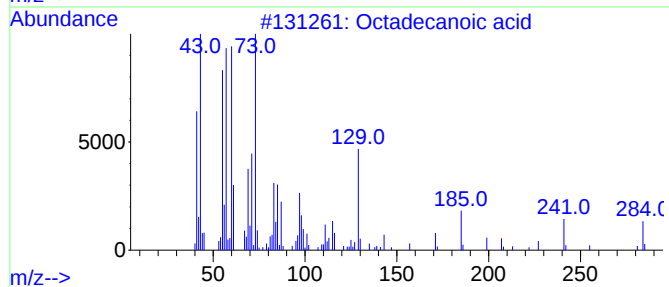
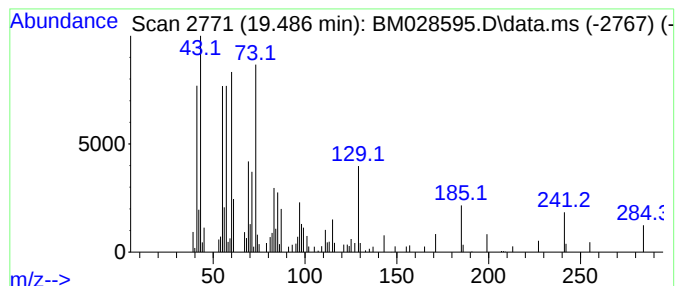
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.486	4.85 ng	92697	Chrysene-d12	21.480

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	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



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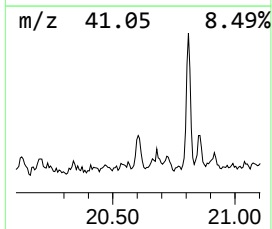
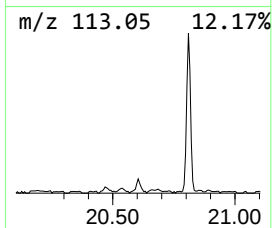
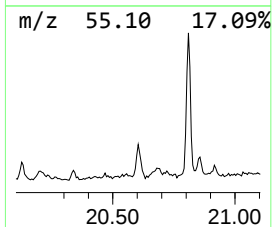
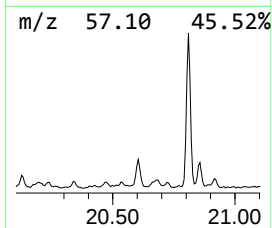
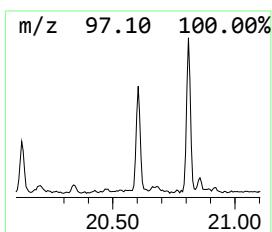
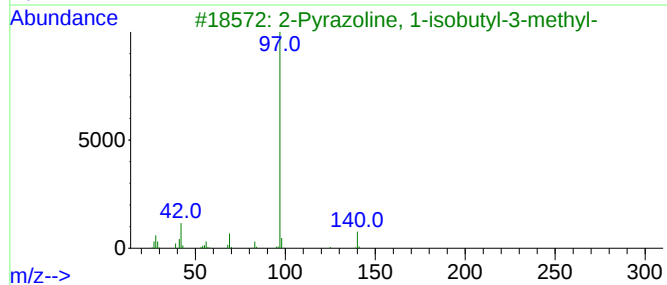
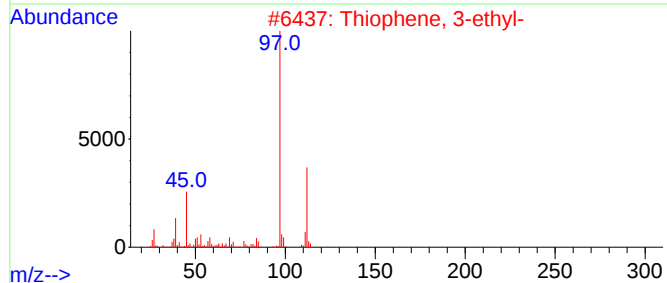
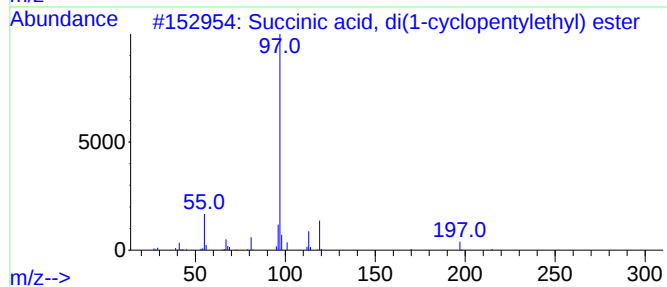
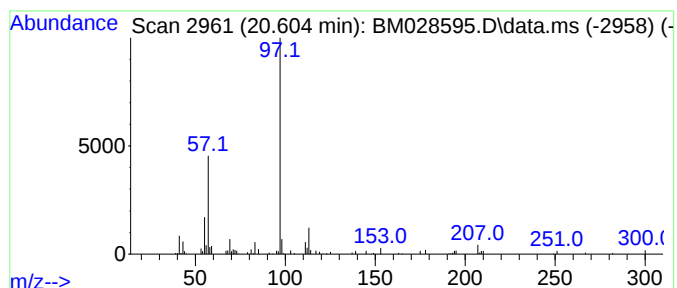
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Succinic acid, di(1-cyclope... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.604	2.26 ng	43245	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, di(1-cyclopentyle...	310	C18H30O4	1000330-21-8	64
2			Thiophene, 3-ethyl-	112	C6H8S	001795-01-3	53
3			2-Pyrazoline, 1-isobutyl-3-methyl-	140	C8H16N2	026964-53-4	53
4			1,2,4-Oxadiazol-5-amine, 3-(4-am...	264	C9H8N6O2S	1000351-26-9	45
5			Methylphosphonic acid, dinonyl e...	348	C19H41O3P	095428-88-9	42



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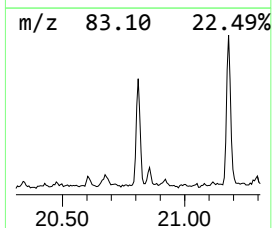
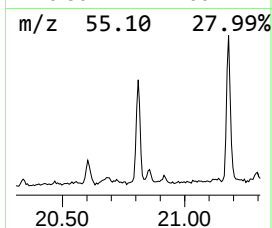
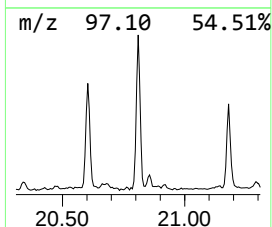
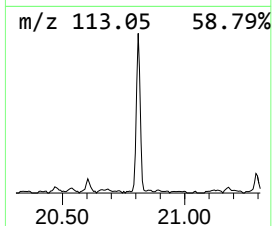
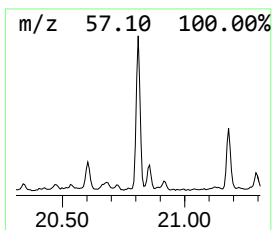
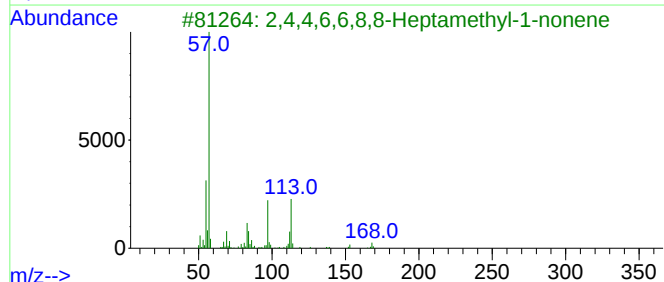
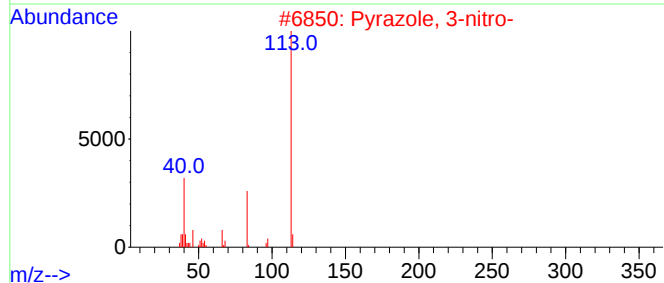
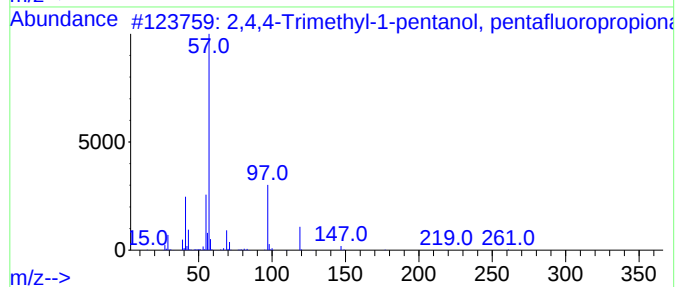
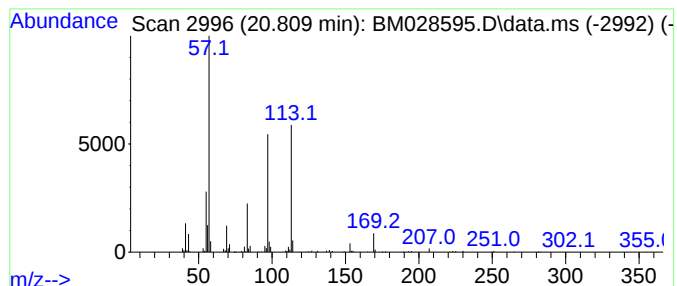
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown20.809 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.809	6.82 ng	130405	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	38		
2	Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	35		
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	32		
4	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	32		
5	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	32		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028595.D
Acq On : 28 Jan 2021 19:46
Operator : CG/JU
Sample : M1255-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CRT-3

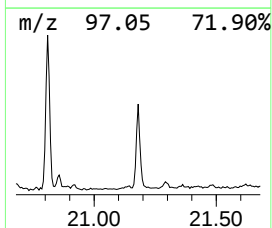
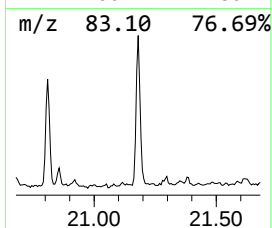
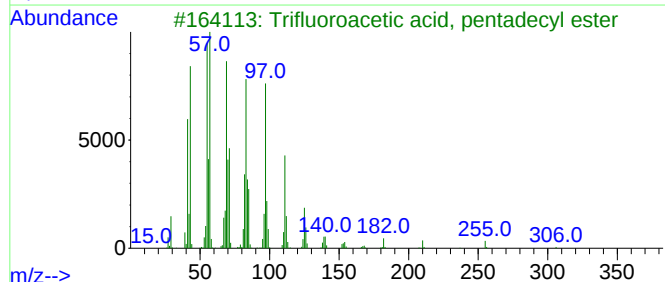
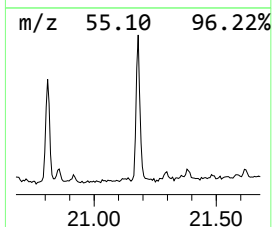
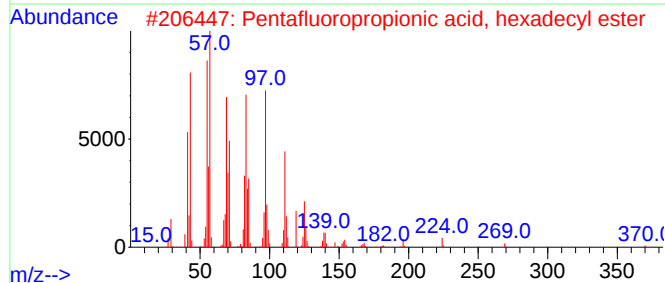
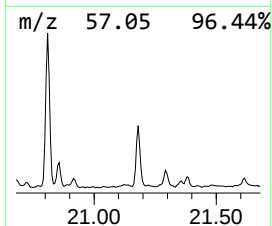
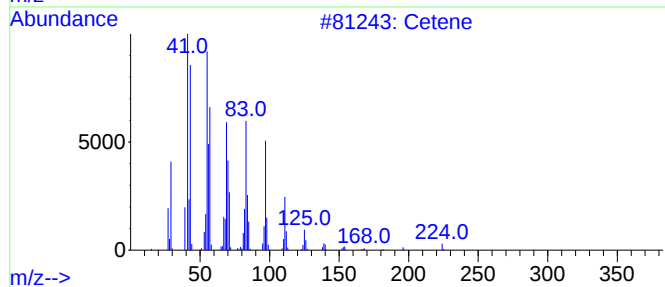
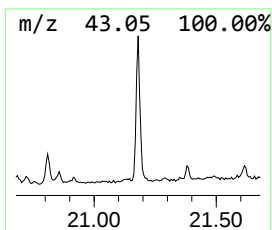
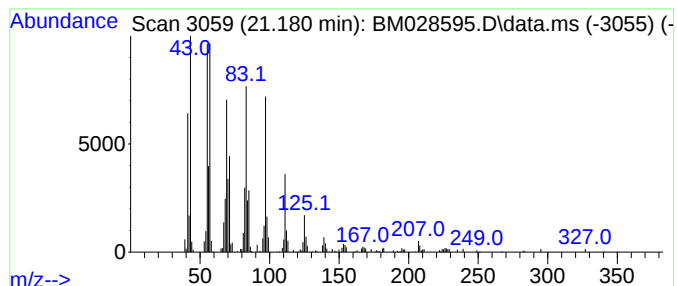
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cetene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	8.50 ng	162587	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cetene	224	C16H32	000629-73-2	94
2			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	94
3			Trifluoroacetic acid, pentadecyl ester	324	C17H31F3O2	959010-23-2	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5			Heptafluorobutyric acid, pentadecyl ester	424	C19H31F7O2	959261-23-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028595.D
Acq On : 28 Jan 2021 19:46
Operator : CG/JU
Sample : M1255-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CRT-3

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.221	10.9	ng	179501	4	17.339	328355	20.0
unknown18.968	18.968	6.9	ng	112618	4	17.339	328355	20.0
Octadecanoic acid	19.486	4.8	ng	92697	5	21.480	382375	20.0
Succinic acid, ...	20.604	2.3	ng	43245	5	21.480	382375	20.0
unknown20.809	20.809	6.8	ng	130405	5	21.480	382375	20.0
Cetene	21.180	8.5	ng	162587	5	21.480	382375	20.0