

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
 Data File : BM028578.D
 Acq On : 27 Jan 2021 20:22
 Operator : CG/JU
 Sample : M1238-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 HD-02-012621

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: BM028578.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	305	312	320	rBV2	6914	10803	1.17%	0.175%
2	5.522	390	397	404	rBV	336668	492850	53.46%	7.988%
3	7.163	670	676	691	rBV	317203	544043	59.02%	8.818%
4	7.969	807	813	819	rBV	97028	151576	16.44%	2.457%
5	9.139	1004	1012	1022	rBV	204803	328285	35.61%	5.321%
6	10.781	1284	1291	1299	rVB	126560	205300	22.27%	3.327%
7	13.233	1702	1708	1715	rBV	461279	662926	71.91%	10.745%
8	14.069	1845	1850	1855	rVB	9509	13158	1.43%	0.213%
9	14.610	1935	1942	1949	rBV2	171271	249331	27.05%	4.041%
10	16.098	2189	2195	2207	rVB	365860	508071	55.11%	8.235%
11	17.086	2351	2363	2367	rBV5	5156	9894	1.07%	0.160%
12	17.345	2401	2407	2412	rBV	209478	290214	31.48%	4.704%
13	17.710	2463	2469	2477	rBV6	5358	10791	1.17%	0.175%
14	17.998	2514	2518	2522	rVB	20078	23990	2.60%	0.389%
15	18.109	2531	2537	2542	rBV3	7396	12489	1.35%	0.202%
16	18.221	2551	2556	2565	rBV	103710	150113	16.28%	2.433%
17	18.509	2600	2605	2611	rBV5	7500	15212	1.65%	0.247%
18	18.709	2636	2639	2645	rVB	8228	13505	1.47%	0.219%
19	18.974	2678	2684	2688	rBV	52718	69252	7.51%	1.122%
20	19.062	2694	2699	2706	rBV	16421	24883	2.70%	0.403%
21	19.127	2706	2710	2713	rBV3	28513	38209	4.14%	0.619%
22	19.156	2713	2715	2719	rVB	39923	44228	4.80%	0.717%
23	19.380	2749	2753	2766	rVV2	30762	67399	7.31%	1.092%
24	19.492	2768	2772	2783	rVV	52000	85247	9.25%	1.382%
25	19.604	2787	2791	2795	rVB	16407	19462	2.11%	0.315%
26	19.745	2811	2815	2823	rVB2	17532	25775	2.80%	0.418%
27	19.939	2843	2848	2854	rBV	739672	921841	100.00%	14.941%
28	20.127	2878	2880	2886	rVB	8738	10439	1.13%	0.169%
29	20.233	2896	2898	2902	rVB2	9726	9909	1.07%	0.161%
30	20.603	2958	2961	2968	rVB	19235	28919	3.14%	0.469%
31	20.809	2992	2996	3000	rBV	67903	77604	8.42%	1.258%
32	20.856	3001	3004	3008	rVB	15499	16407	1.78%	0.266%
33	21.180	3055	3059	3064	rBV	127536	159508	17.30%	2.585%
34	21.480	3106	3110	3115	rBV	285329	386215	41.90%	6.260%
35	23.744	3490	3495	3504	rVB2	190641	366501	39.76%	5.940%
36	24.256	3579	3582	3591	rVB	73609	125511	13.62%	2.034%

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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

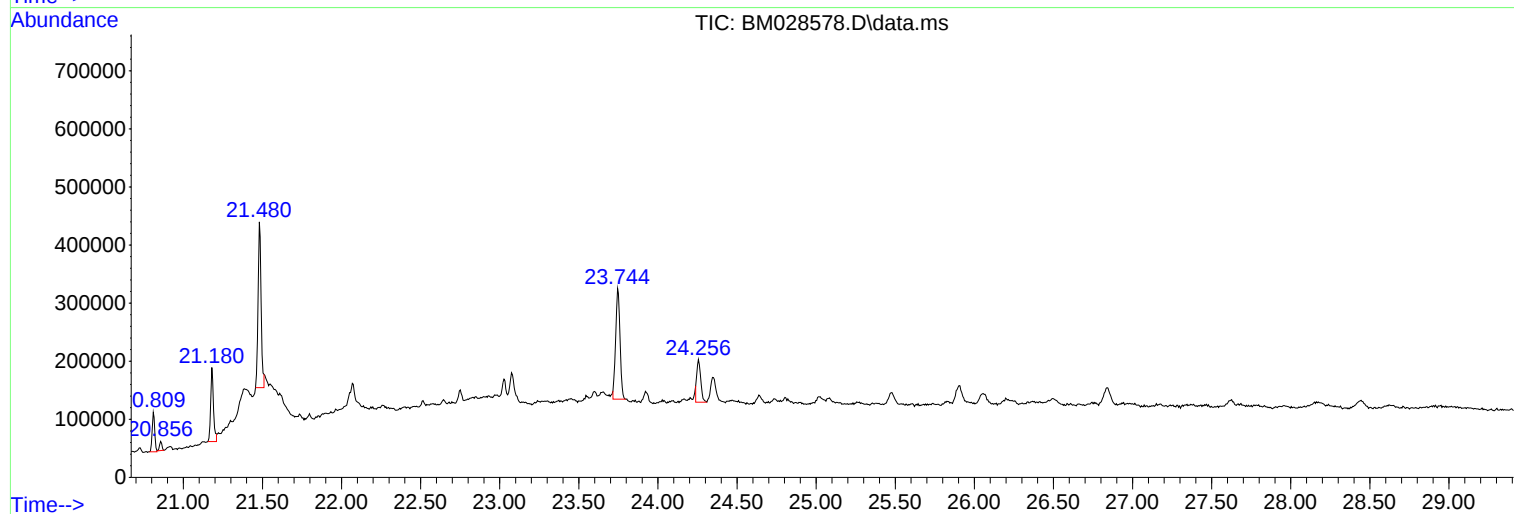
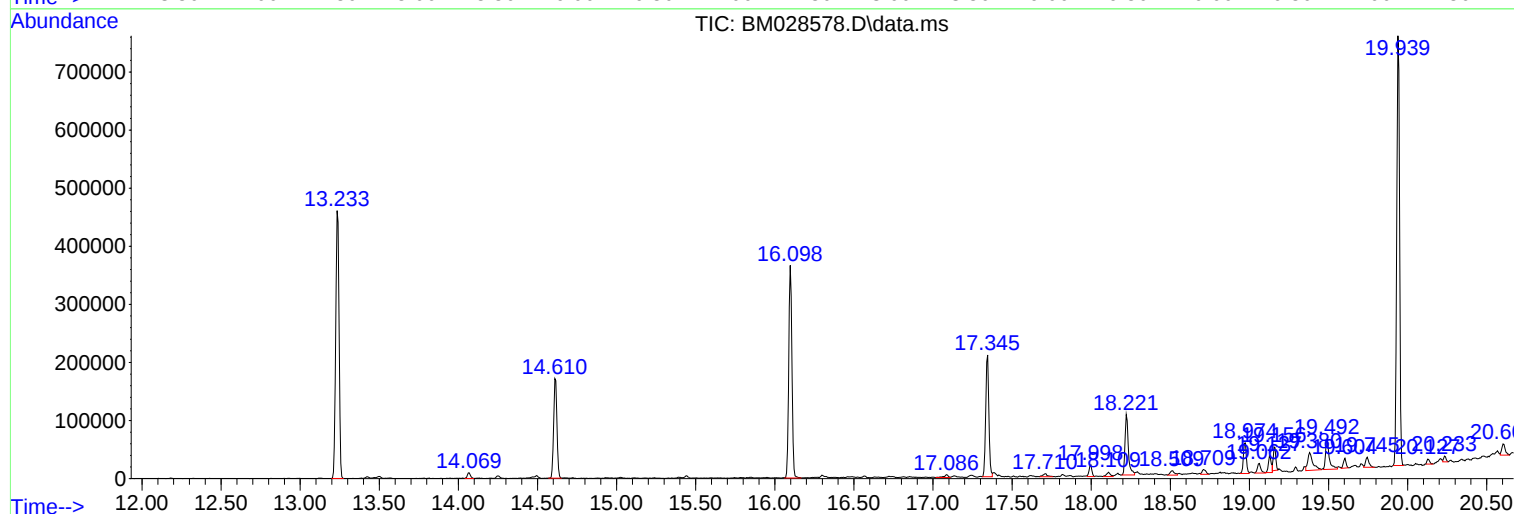
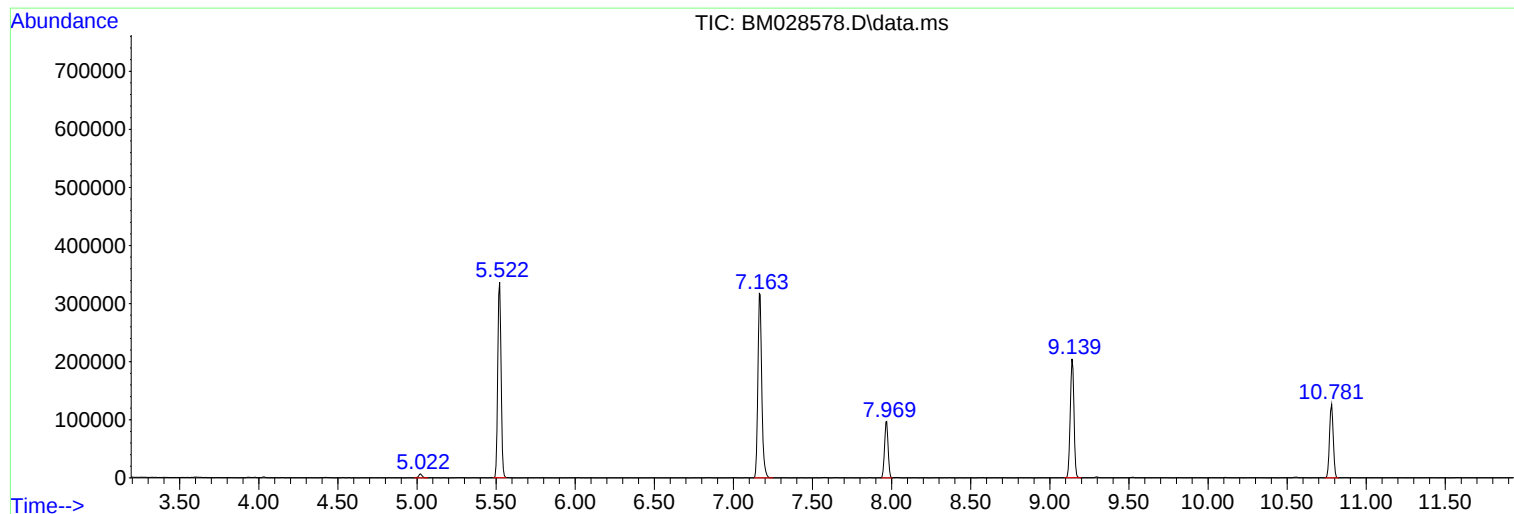
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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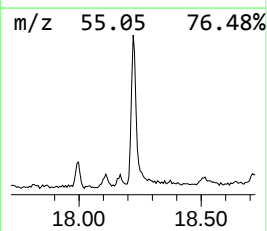
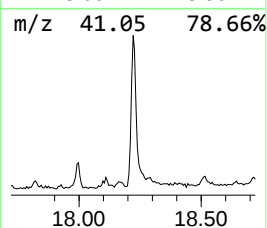
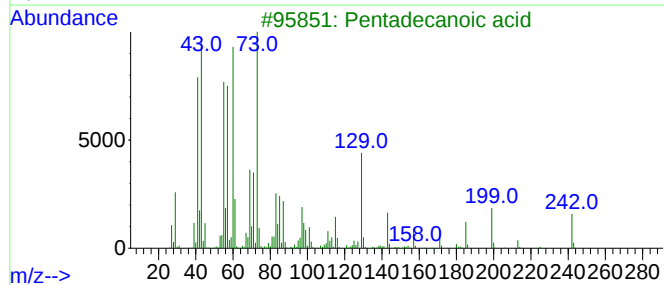
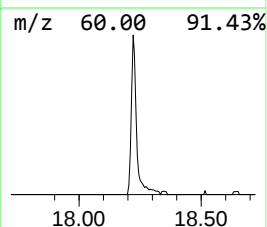
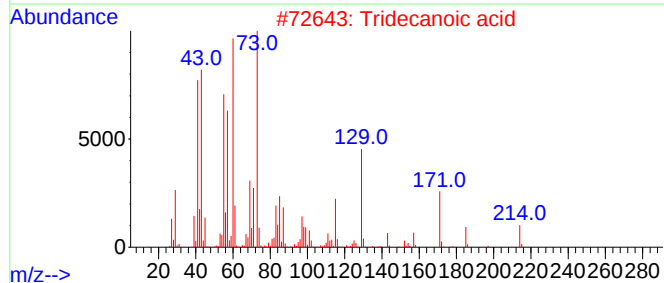
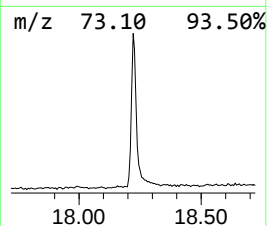
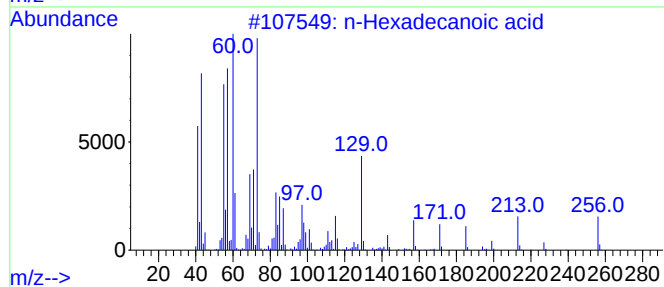
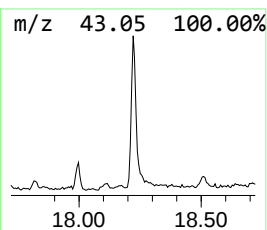
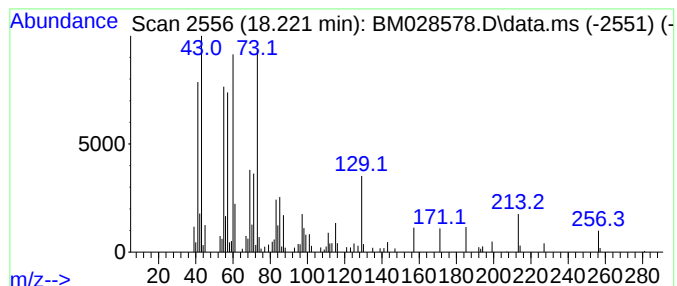
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.221	10.35 ng	150113	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	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Isopropyl palmitate	298	C19H38O2	000142-91-6	64



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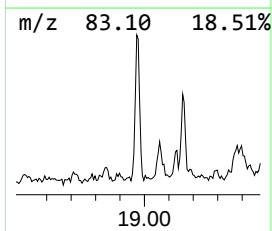
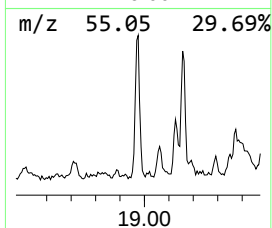
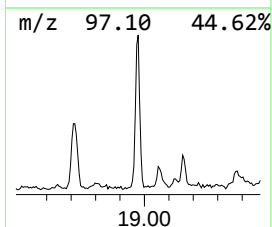
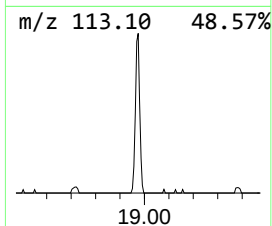
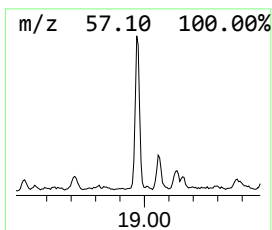
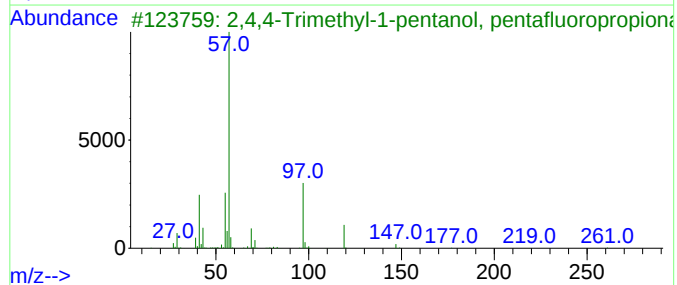
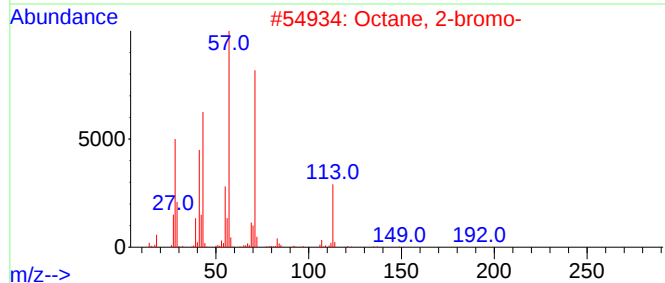
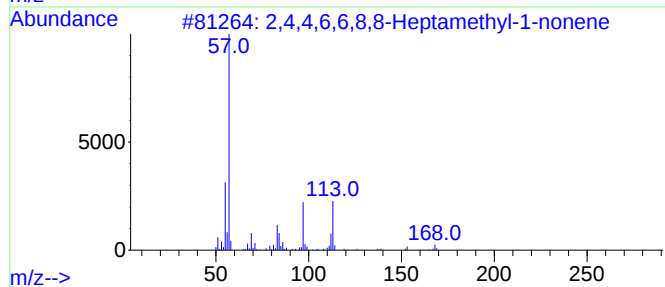
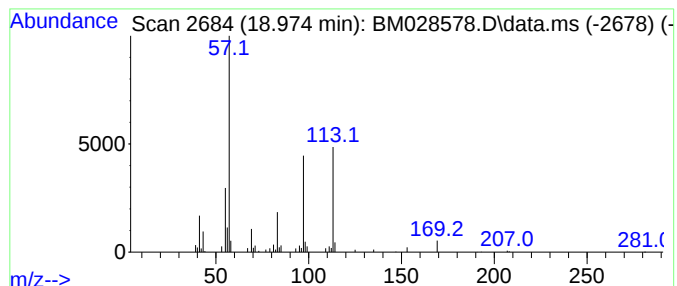
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Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.974	4.77 ng	69252	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	72		
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	47		
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	37		
4	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	35		
5	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	32		



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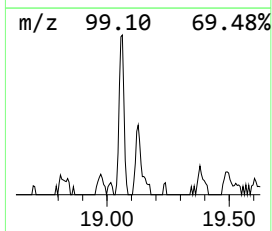
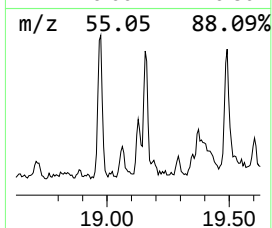
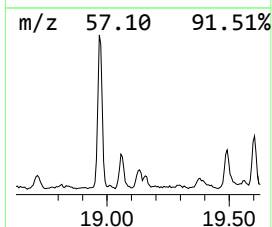
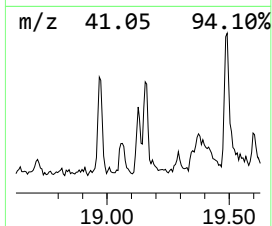
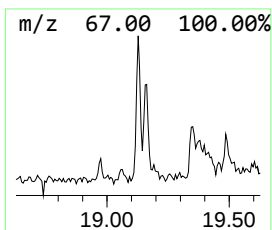
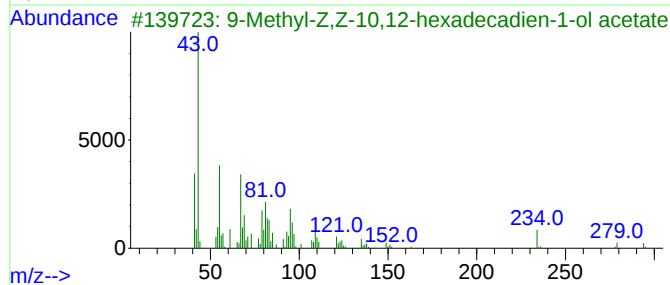
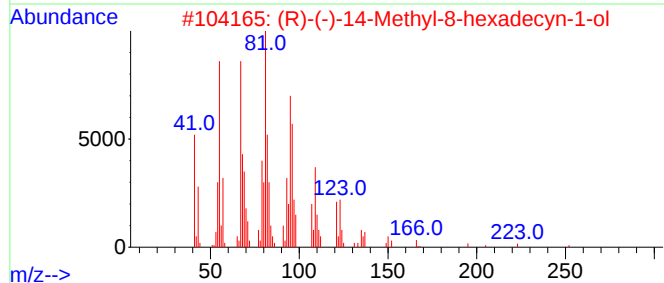
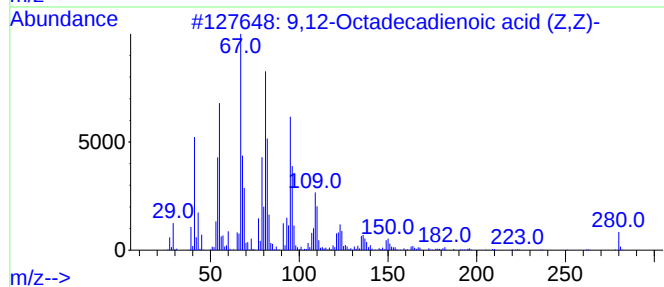
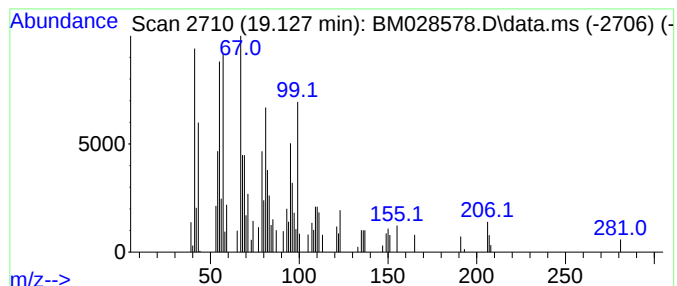
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9,12-Octadecadienoic acid (... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.127	2.63 ng	38209	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	76
2			(R)-(-)-14-Methyl-8-hexadecyn-1-ol	252	C17H32O	064566-18-3	70
3			9-Methyl-Z,Z-10,12-hexadecadien-...	294	C19H34O2	1000130-89-6	64
4			Ethanol, 2-(9,12-octadecadienyl)-...	310	C20H38O2	017367-08-7	60
5			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	58



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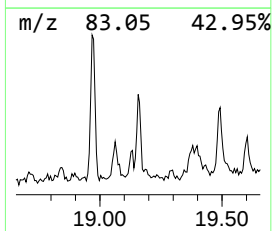
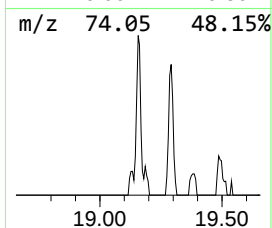
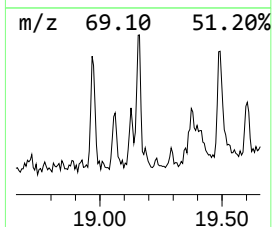
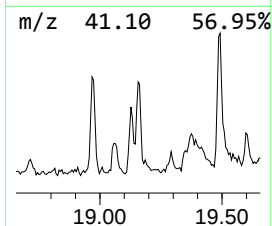
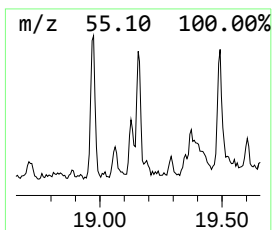
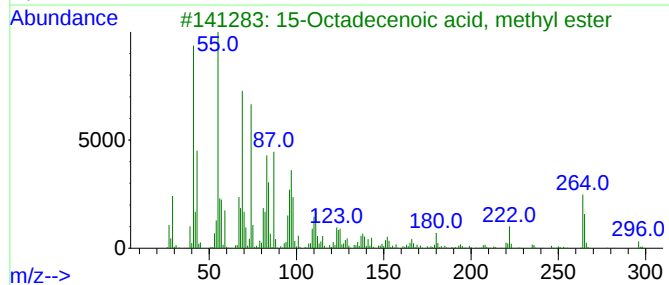
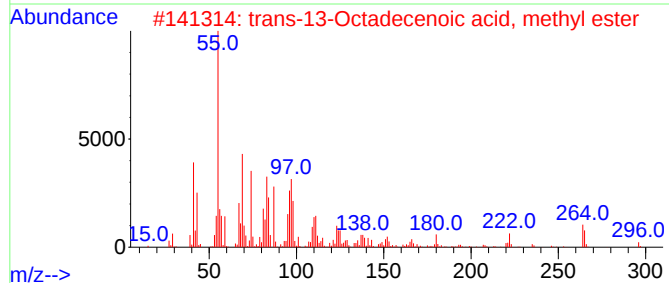
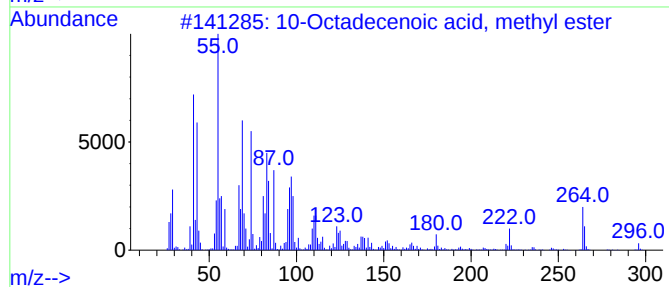
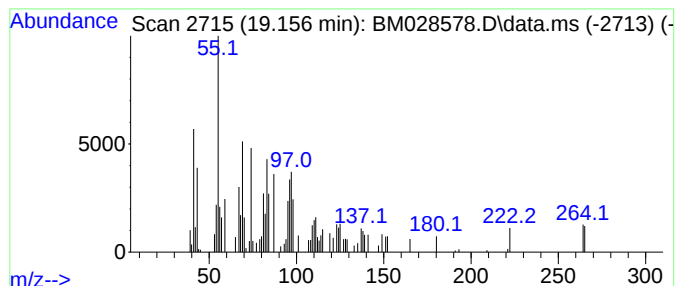
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 10-Octadecenoic acid, methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.157	3.05 ng	44228	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
2			trans-13-Octadecenoic acid, methyl ester	296	C19H36O2	1000333-61-3	91
3			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
4			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
5			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	90



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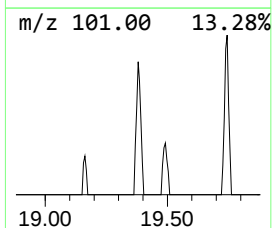
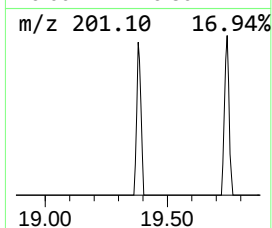
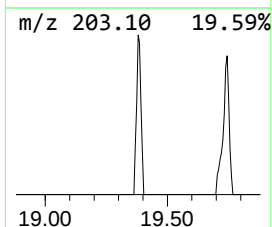
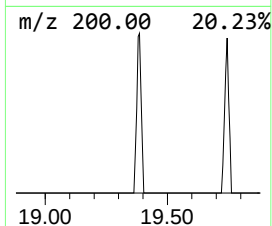
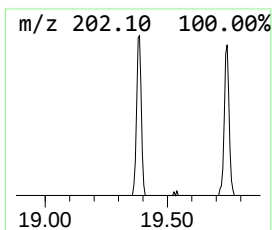
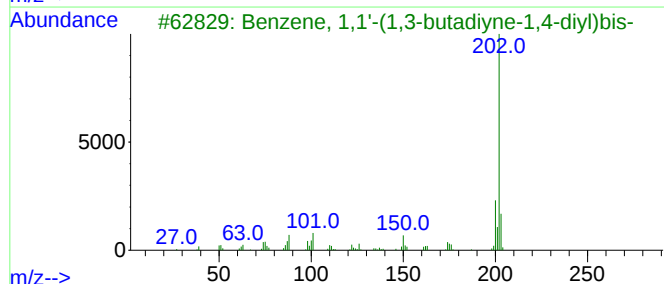
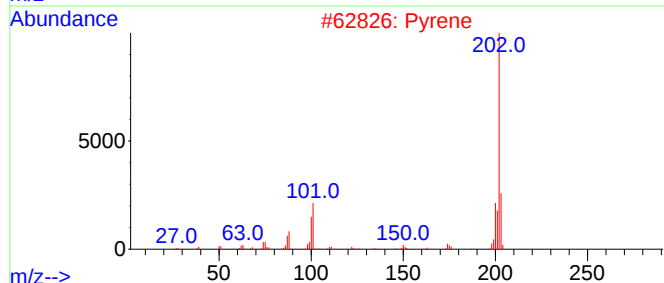
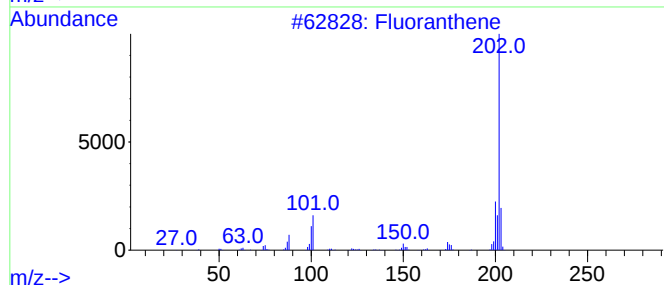
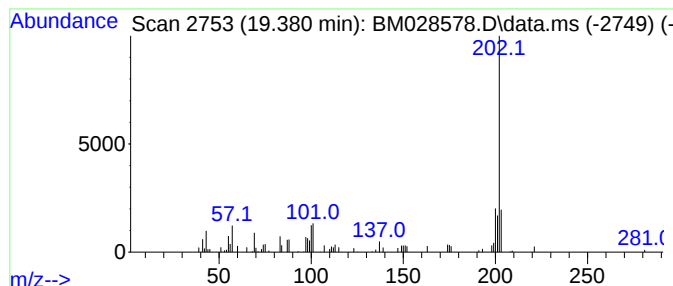
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.380	4.64 ng	67399	Phenanthrene-d10	17.345	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	94
2	Pyrene	202	C16H10	000129-00-0	87
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	81
4	1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	56
5	Anthracene, 9-(2-nitroethenyl)-	249	C16H11NO2	058349-77-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028578.D
Acq On : 27 Jan 2021 20:22
Operator : CG/JU
Sample : M1238-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HD-02-012621

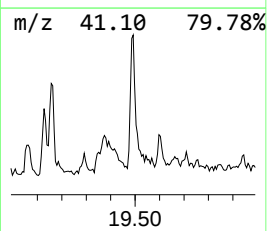
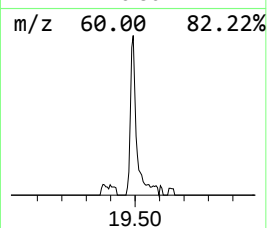
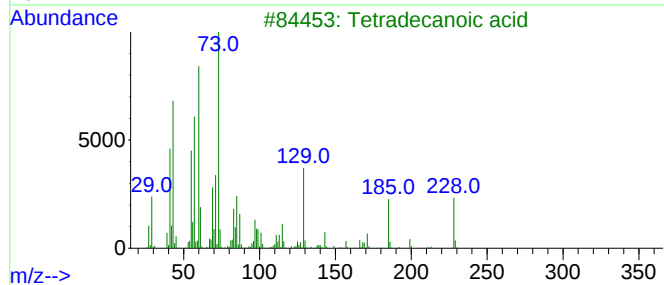
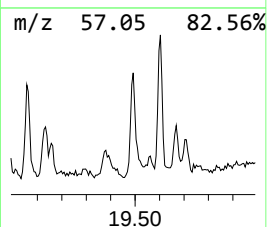
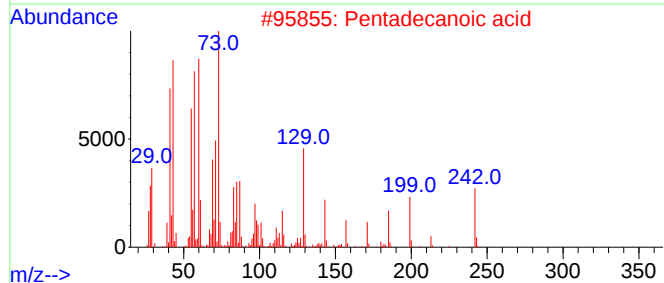
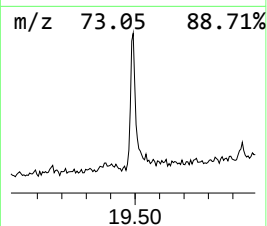
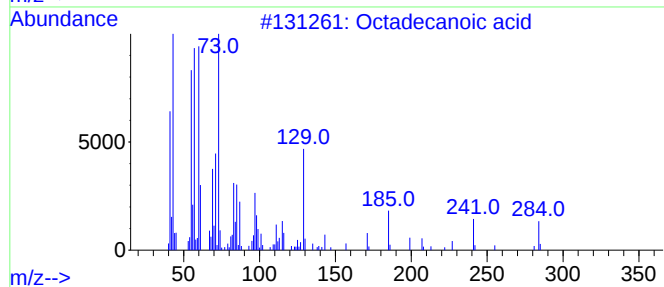
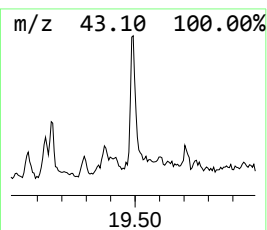
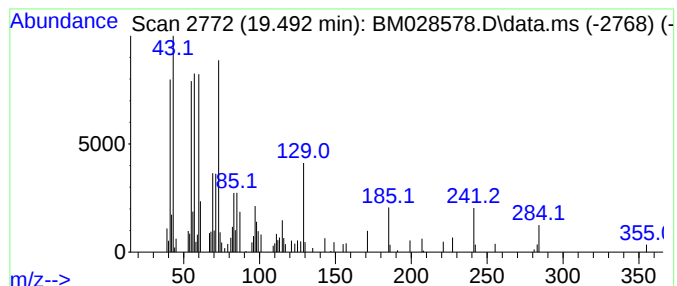
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.492	4.41 ng	85247	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
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Operator : CG/JU
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ClientSampleId :
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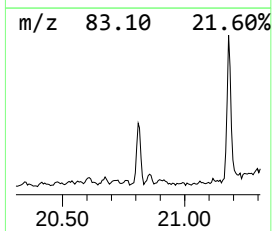
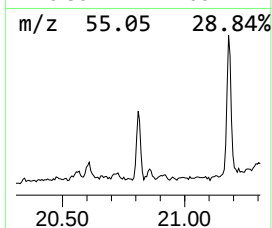
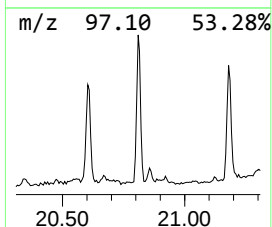
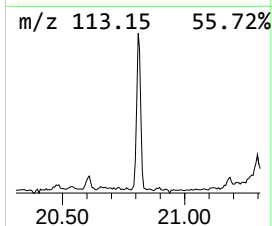
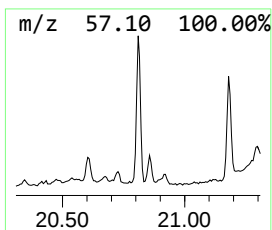
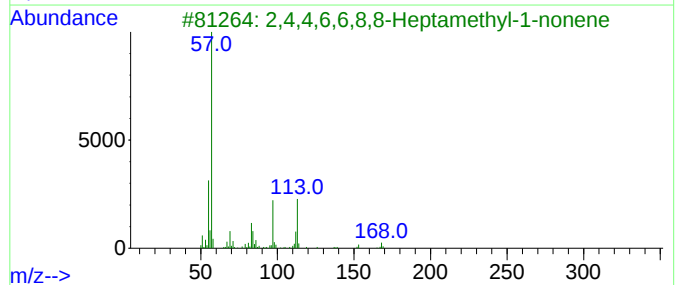
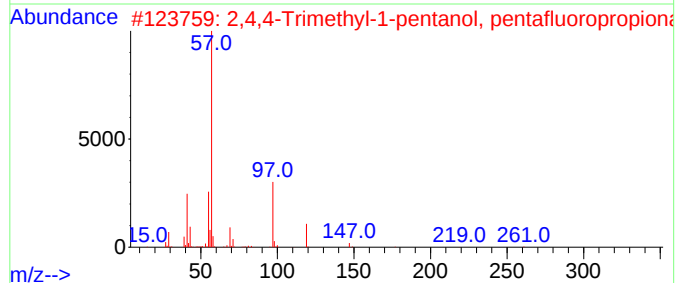
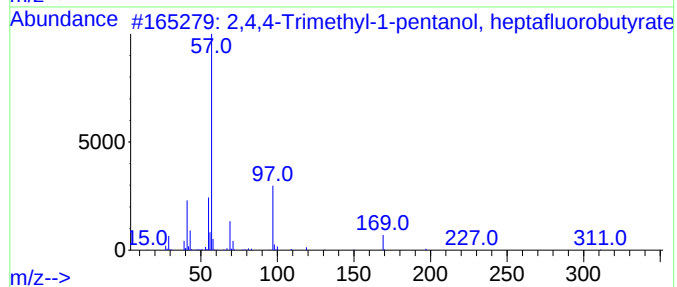
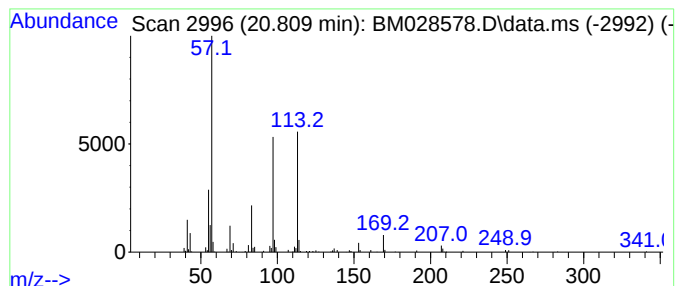
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown20.809 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.809	4.02 ng	77604	Chrysene-d12	21.480

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	35	
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	25	
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	25	
4	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	25	
5	6H-Pyrido[2,3-b][1,4]benzodiazep...	351	C19H21N5O2	028797-61-7	22	



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Sample : M1238-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

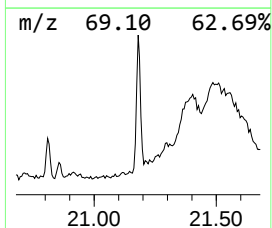
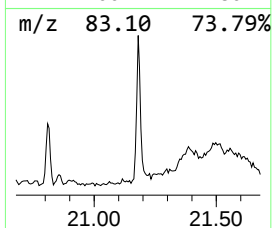
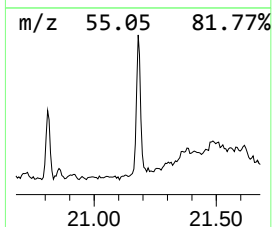
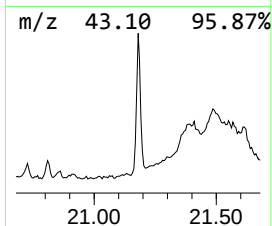
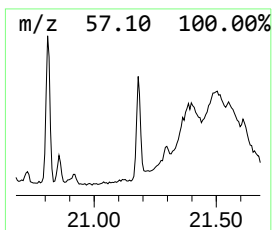
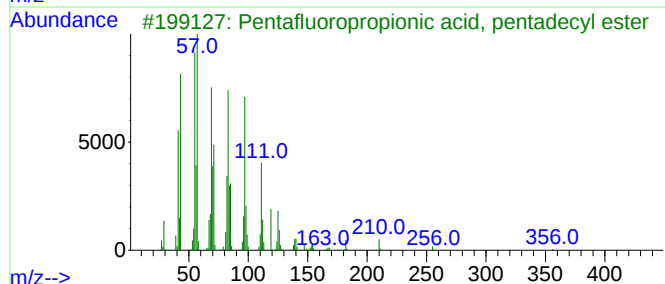
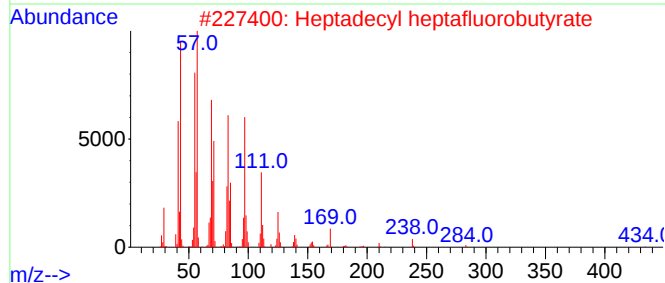
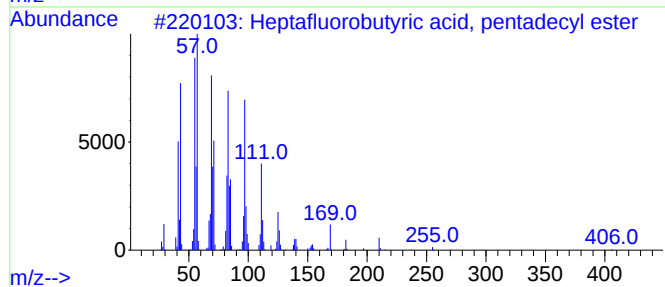
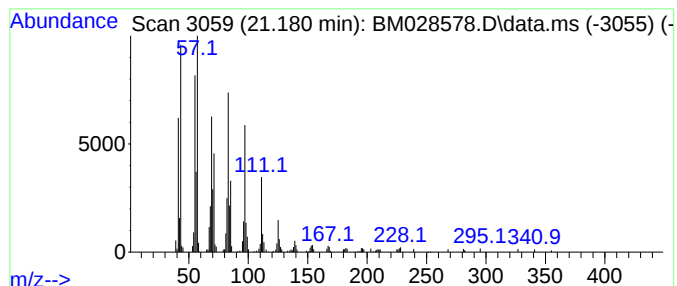
Instrument :
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ClientSampleId :
HD-02-012621

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 8 Heptafluorobutyric acid, pe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.180	8.26 ng	159508	Chrysene-d12	21.480	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Cyclotetracosane	336	C24H48	000297-03-0	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93



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Sample : M1238-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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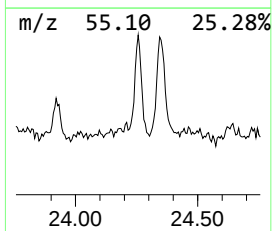
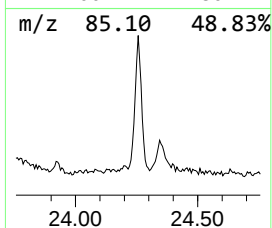
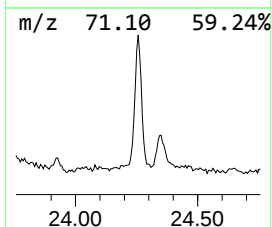
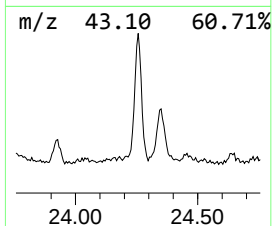
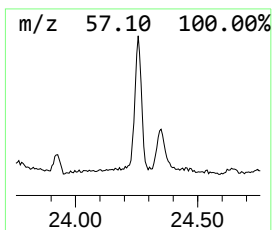
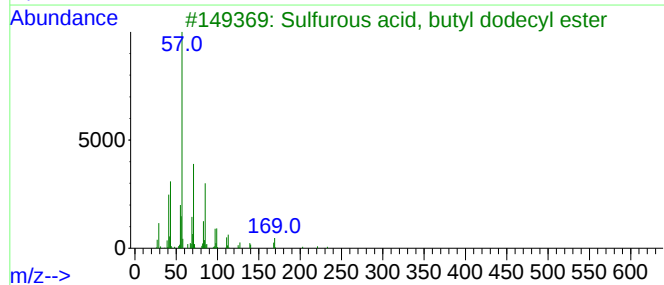
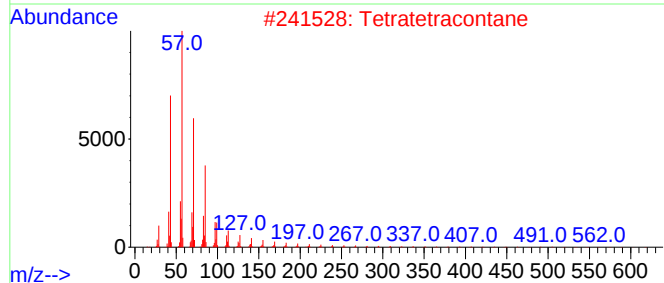
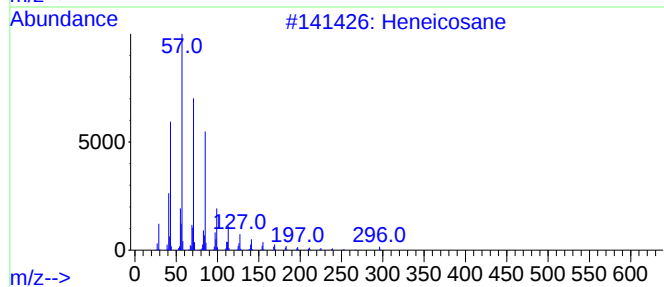
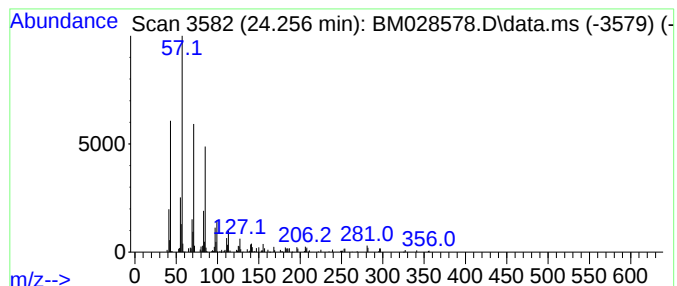
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.256	6.85 ng	125511	Perylene-d12	23.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	98
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	91
4			Octadecane	254	C18H38	000593-45-3	89
5			2-methyloctacosane	408	C29H60	1000376-72-8	87



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Sample : M1238-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.221	10.4	ng	150113	4	17.345	290214	20.0
2,4,4,6,6,8,8-H...	18.974	4.8	ng	69252	4	17.345	290214	20.0
9,12-Octadecadi...	19.127	2.6	ng	38209	4	17.345	290214	20.0
10-Octadecenoic...	19.157	3.0	ng	44228	4	17.345	290214	20.0
Benzene, 1,1'-(...	19.380	4.6	ng	67399	4	17.345	290214	20.0
Octadecanoic acid	19.492	4.4	ng	85247	5	21.480	386215	20.0
unknown20.809	20.809	4.0	ng	77604	5	21.480	386215	20.0
Heptafluorobuty...	21.180	8.3	ng	159508	5	21.480	386215	20.0
Heneicosane	24.256	6.8	ng	125511	6	23.744	366501	20.0