

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081023\
 Data File : BM041368.D
 Acq On : 10 Aug 2023 18:25
 Operator : MA/JU
 Sample : 03955-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-22

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-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041368.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	286	290	299	rVB	25118	39524	1.30%	0.166%
2	5.351	361	368	384	rBV	1064630	1639150	53.84%	6.868%
3	6.957	634	641	665	rBV	839345	1533149	50.36%	6.424%
4	7.775	772	780	789	rBV	427721	689916	22.66%	2.891%
5	8.951	972	980	1000	rBV	525308	1000041	32.85%	4.190%
6	10.580	1249	1257	1263	rBV	479576	846605	27.81%	3.547%
7	10.627	1263	1265	1276	rVB	52443	89325	2.93%	0.374%
8	13.057	1672	1678	1703	rBV	1322666	2129192	69.94%	8.921%
9	14.439	1906	1913	1921	rBV	572110	982417	32.27%	4.116%
10	14.504	1921	1924	1940	rVB	63259	132063	4.34%	0.553%
11	14.857	1977	1984	1992	rBV2	22900	62738	2.06%	0.263%
12	15.504	2087	2094	2106	rBV2	33325	69402	2.28%	0.291%
13	15.945	2163	2169	2183	rBV	946217	1552432	51.00%	6.505%
14	16.945	2333	2339	2345	rBV8	19246	40802	1.34%	0.171%
15	17.027	2348	2353	2360	rVB	25893	42915	1.41%	0.180%
16	17.204	2377	2383	2387	rBV	791870	1188126	39.03%	4.978%
17	17.245	2387	2390	2399	rVV	493397	720228	23.66%	3.018%
18	17.339	2400	2406	2411	rVV	86046	142978	4.70%	0.599%
19	17.633	2449	2456	2462	rBV2	29832	68759	2.26%	0.288%
20	18.103	2528	2536	2540	rBV2	425385	692687	22.75%	2.902%
21	18.221	2553	2556	2560	rVB	27789	37226	1.22%	0.156%
22	18.280	2561	2566	2570	rVV2	71412	122069	4.01%	0.511%
23	18.315	2570	2572	2579	rVB	39733	55407	1.82%	0.232%
24	18.592	2615	2619	2625	rBV	38869	51320	1.69%	0.215%
25	18.651	2626	2629	2634	rVB5	21854	31382	1.03%	0.131%
26	19.009	2685	2690	2695	rBV3	30402	67097	2.20%	0.281%
27	19.156	2710	2715	2721	rVB5	22147	47825	1.57%	0.200%
28	19.274	2728	2735	2743	rBV	650791	917199	30.13%	3.843%
29	19.386	2749	2754	2768	rBV2	232423	453797	14.91%	1.901%
30	19.609	2787	2792	2793	rBV2	112534	146392	4.81%	0.613%
31	19.639	2793	2797	2805	rVV	529212	747505	24.55%	3.132%
32	19.709	2807	2809	2816	rVB4	36593	54278	1.78%	0.227%
33	19.839	2825	2831	2838	rBV	2440408	3044216	100.00%	12.756%
34	20.139	2879	2882	2887	rVB	71280	88707	2.91%	0.372%
35	20.409	2925	2928	2930	rBV2	39576	53283	1.75%	0.223%
36	21.109	3044	3047	3057	rVB4	243049	348911	11.46%	1.462%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081023\
Data File : BM041368.D
Acq On : 10 Aug 2023 18:25
Operator : MA/JU
Sample : 03955-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-22

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-BM072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.409	3091	3098	3102	rBV2	1296005	2039167	66.98%	8.544%
38	21.444	3102	3104	3112	rVB	272305	320297	10.52%	1.342%
39	23.774	3494	3500	3506	rBV	820383	1577353	51.81%	6.609%

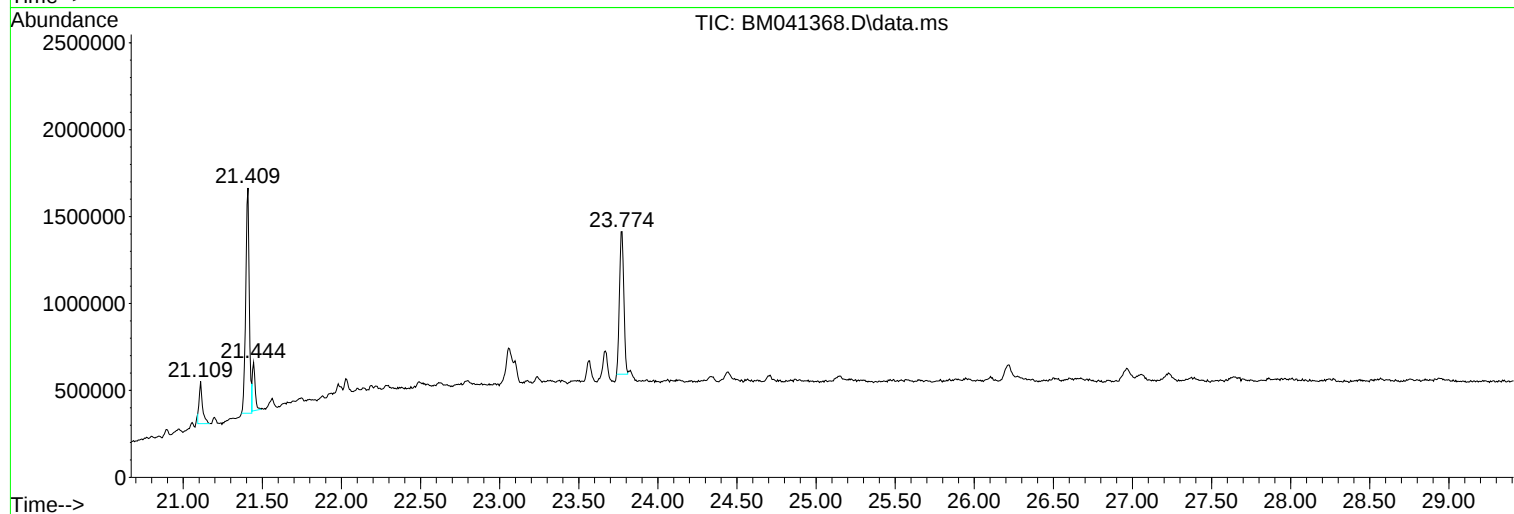
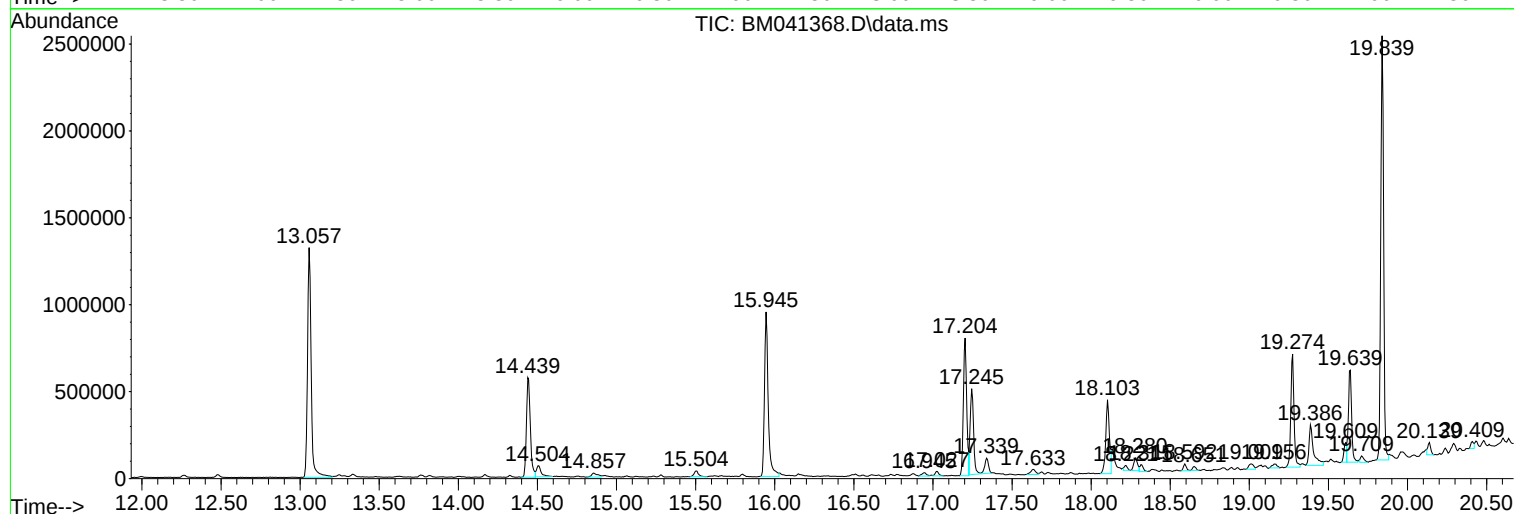
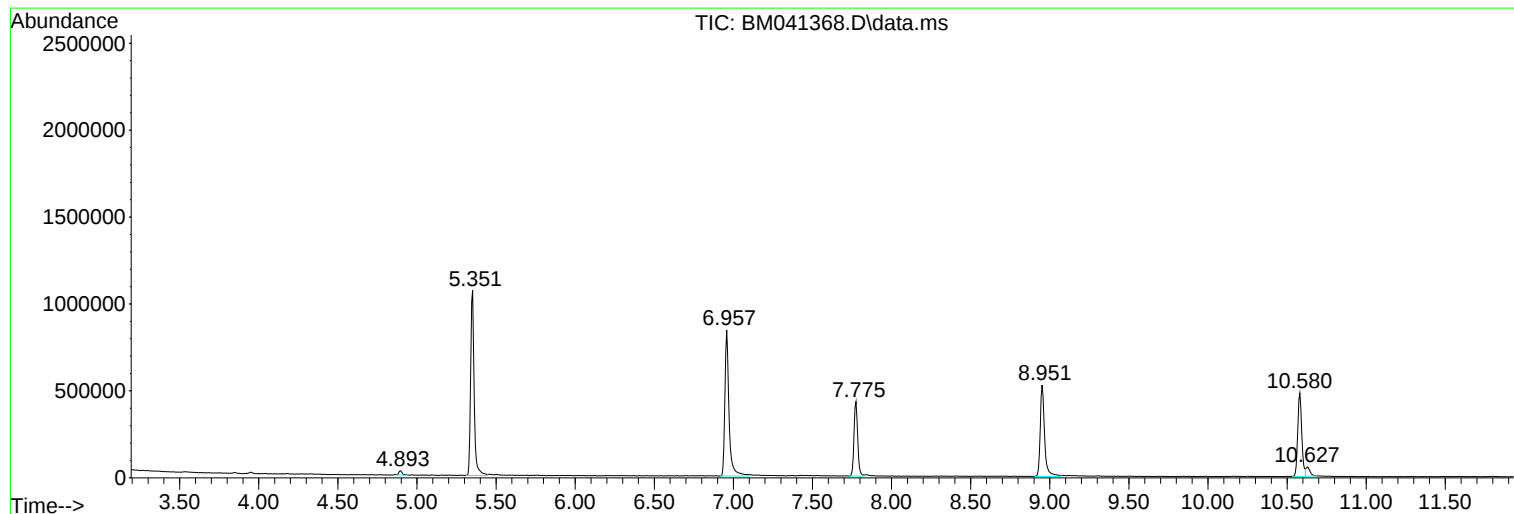
Sum of corrected areas: 23865880

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081023\
Data File : BM041368.D
Acq On : 10 Aug 2023 18:25
Operator : MA/JU
Sample : 03955-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081023\
Data File : BM041368.D
Acq On : 10 Aug 2023 18:25
Operator : MA/JU
Sample : 03955-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-22

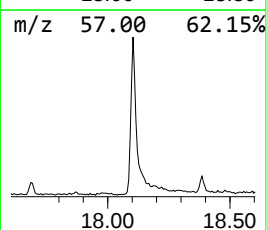
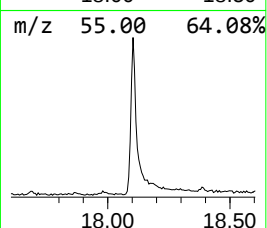
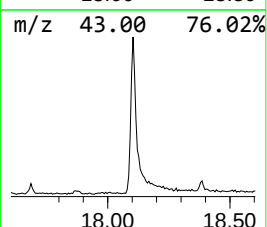
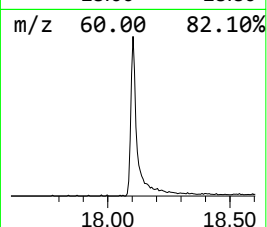
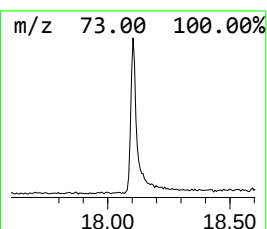
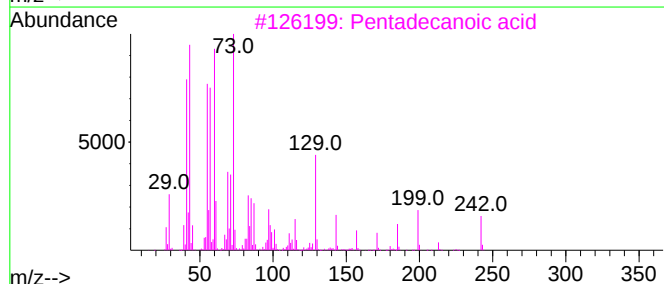
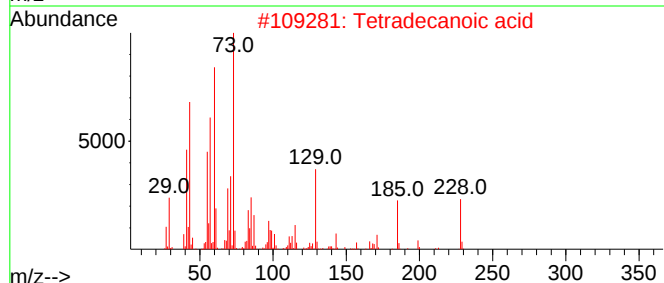
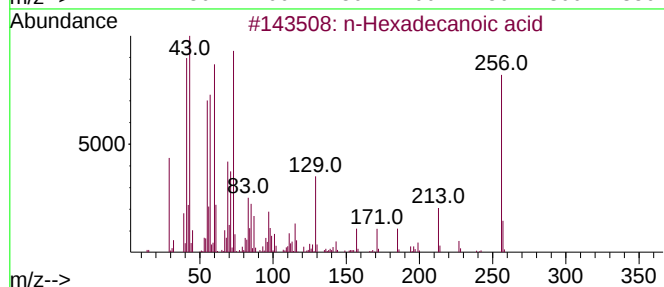
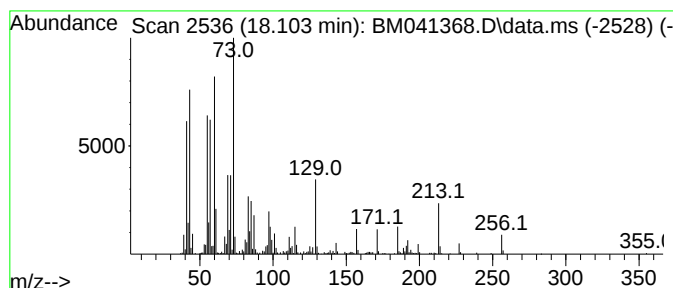
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	11.66 ng	692687	Phenanthrene-d10	17.203

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	74
5			Octadecanoic acid	284	C18H36O2	000057-11-4	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081023\
Data File : BM041368.D
Acq On : 10 Aug 2023 18:25
Operator : MA/JU
Sample : 03955-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

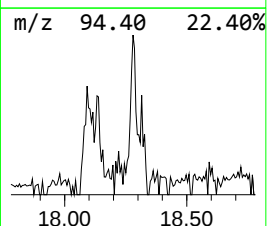
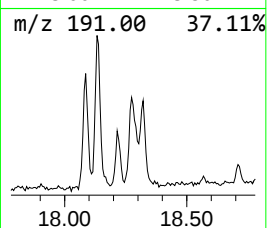
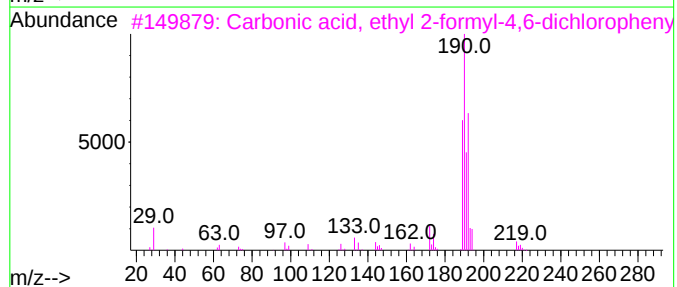
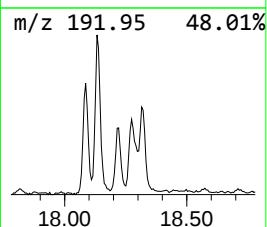
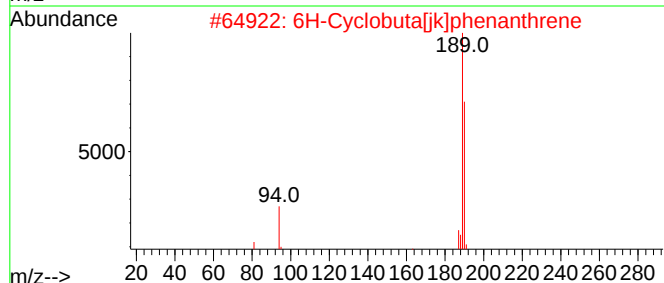
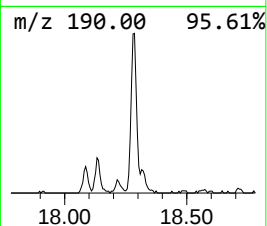
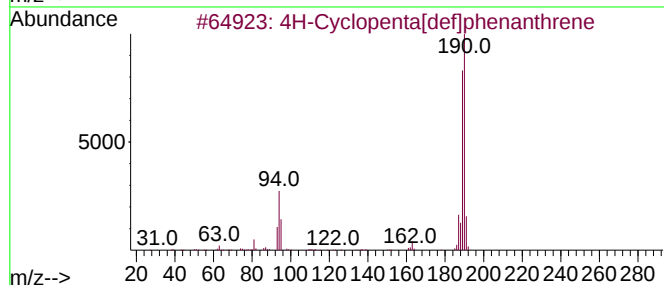
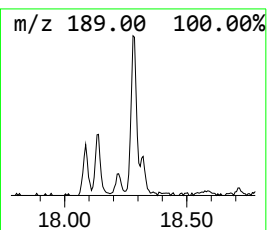
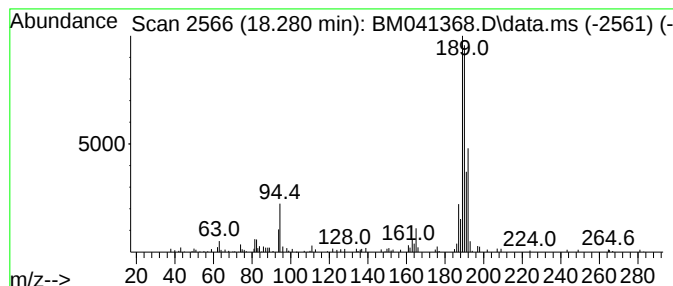
Instrument :
BNA_M
ClientSampleId :
WC-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.280	2.05 ng	122069	Phenanthrene-d10	17.203	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	28
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	28
5	1,2,3,4,5,6,7,8,9,10-Decahydro-5...	190	C13H18O	1000497-99-5	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081023\
Data File : BM041368.D
Acq On : 10 Aug 2023 18:25
Operator : MA/JU
Sample : 03955-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-22

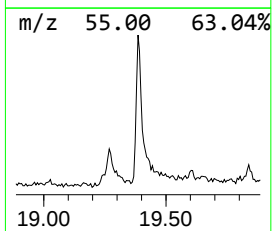
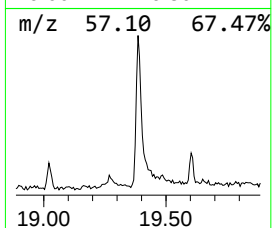
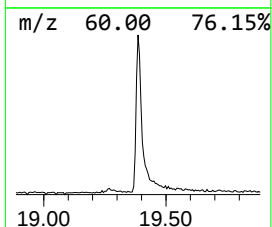
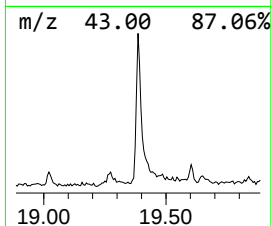
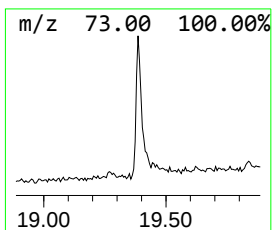
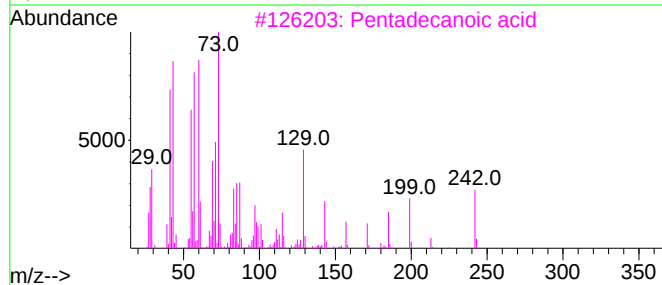
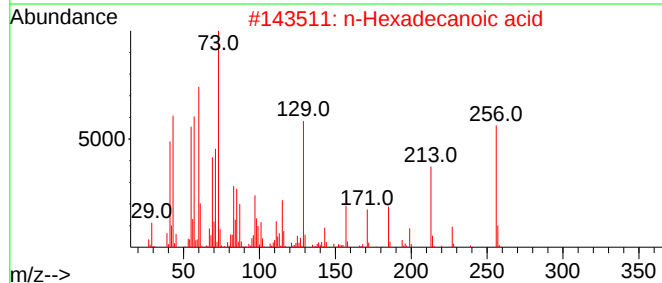
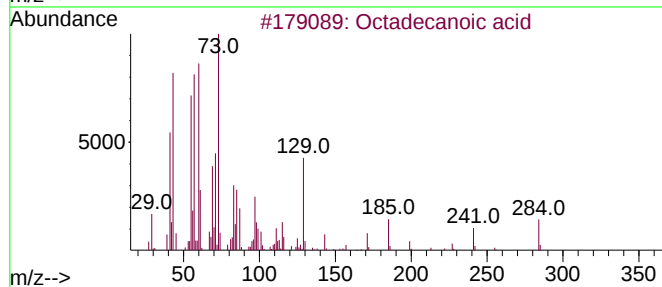
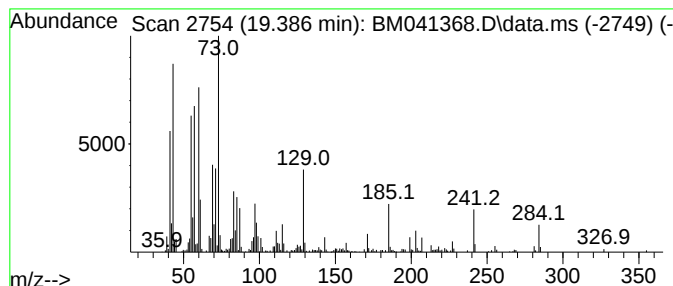
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	4.45 ng	453797	Chrysene-d12	21.409

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081023\
Data File : BM041368.D
Acq On : 10 Aug 2023 18:25
Operator : MA/JU
Sample : 03955-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-22

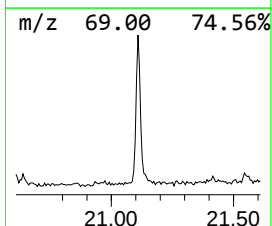
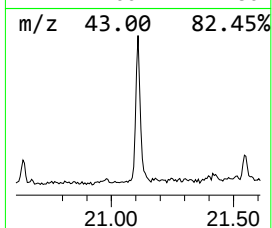
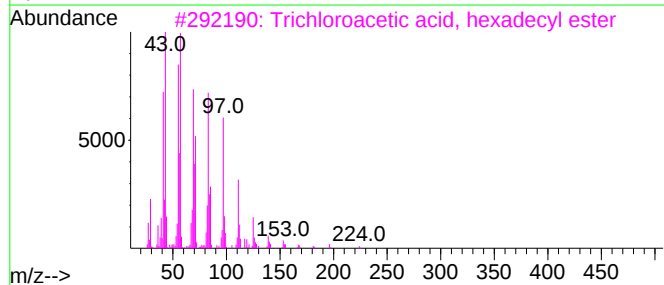
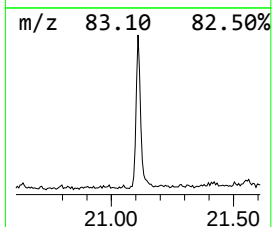
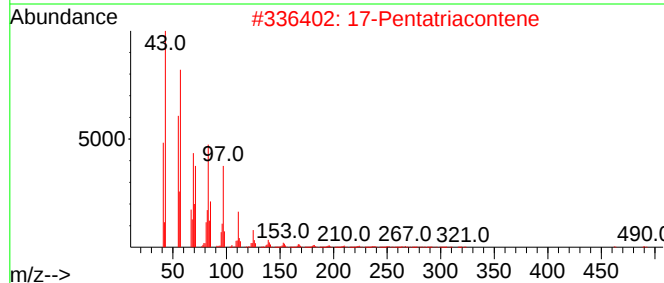
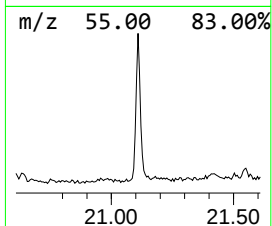
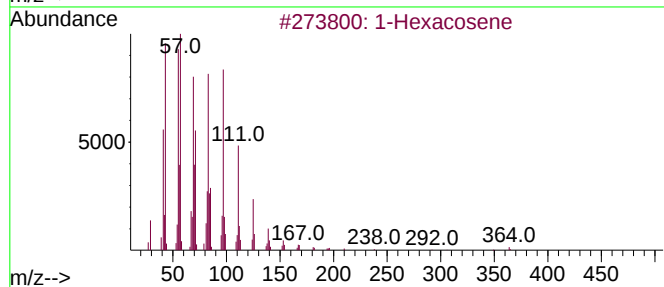
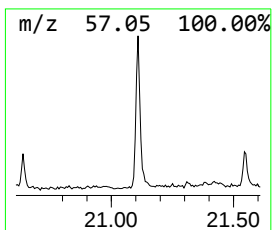
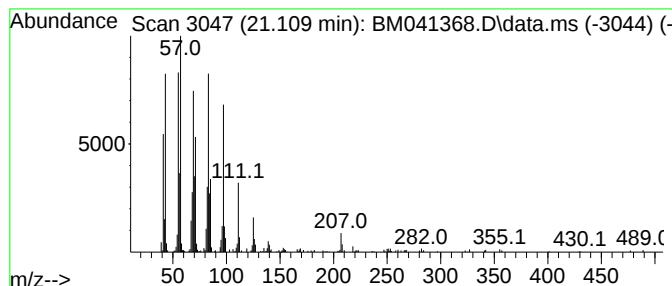
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.109	3.42 ng	348911	Chrysene-d12	21.409

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	94
2			17-Pentatriacontene	491	C35H70	006971-40-0	91
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5			Octacosanol	410	C28H58O	000557-61-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081023\
Data File : BM041368.D
Acq On : 10 Aug 2023 18:25
Operator : MA/JU
Sample : 03955-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.104	11.7	ng	692687	4	17.203	1188130	20.0
4H-Cyclopenta[d...]	18.280	2.0	ng	122069	4	17.203	1188130	20.0
Octadecanoic acid	19.386	4.5	ng	453797	5	21.409	2039170	20.0
1-Hexacosene	21.109	3.4	ng	348911	5	21.409	2039170	20.0