

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
 Data File : BM042441.D
 Acq On : 25 Oct 2023 17:12
 Operator : MA/JU
 Sample : 04941-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 72-12017

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-BM102123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042441.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	316	320	329	rVB	246334	334079	8.28%	0.941%
2	5.522	390	397	410	rBV	1991657	2936481	72.78%	8.273%
3	7.145	665	673	687	rBV	1940902	3129560	77.56%	8.817%
4	7.992	810	817	827	rBV	568239	890500	22.07%	2.509%
5	9.186	1011	1020	1035	rBV	1209835	1994296	49.43%	5.619%
6	10.810	1289	1296	1304	rBV	721791	1193855	29.59%	3.364%
7	13.257	1706	1712	1726	rVB	2254163	3107560	77.02%	8.755%
8	13.480	1744	1750	1756	rBV2	30797	51118	1.27%	0.144%
9	14.633	1939	1946	1954	rBV	1060707	1524296	37.78%	4.295%
10	15.004	2005	2009	2015	rBV4	25014	41520	1.03%	0.117%
11	16.127	2193	2200	2210	rVB	2280612	3197644	79.25%	9.009%
12	16.280	2221	2226	2232	rBV2	22859	42124	1.04%	0.119%
13	17.015	2346	2351	2356	rBV	68760	110949	2.75%	0.313%
14	17.386	2408	2414	2418	rBV	1380632	1882375	46.65%	5.303%
15	17.427	2418	2421	2427	rVB	153826	204387	5.07%	0.576%
16	17.521	2430	2437	2443	rBV	38384	78551	1.95%	0.221%
17	18.233	2552	2558	2567	rBV	1202565	1844151	45.70%	5.196%
18	18.450	2590	2595	2599	rBV2	49209	96473	2.39%	0.272%
19	18.492	2599	2602	2607	rVB2	31657	43617	1.08%	0.123%
20	18.815	2654	2657	2663	rVB4	38874	50943	1.26%	0.144%
21	19.086	2700	2703	2708	rVB5	28217	41026	1.02%	0.116%
22	19.162	2713	2716	2721	rVB2	43314	64627	1.60%	0.182%
23	19.392	2752	2755	2756	rVV	64372	72829	1.80%	0.205%
24	19.439	2758	2763	2768	rVB	470192	666742	16.52%	1.879%
25	19.509	2770	2775	2786	rBV	862971	1313279	32.55%	3.700%
26	19.762	2815	2818	2821	rBV3	68903	94933	2.35%	0.267%
27	19.803	2821	2825	2831	rVB	467121	608258	15.07%	1.714%
28	19.997	2852	2858	2865	rBV	3206269	4034973	100.00%	11.368%
29	20.250	2898	2901	2905	rBV3	70901	99931	2.48%	0.282%
30	20.286	2905	2907	2912	rVB	66673	91971	2.28%	0.259%
31	20.744	2983	2985	2988	rBV	54594	46477	1.15%	0.131%
32	21.221	3061	3066	3074	rBV4	374898	733900	18.19%	2.068%
33	21.562	3118	3124	3129	rBV2	1723565	2528196	62.66%	7.123%
34	21.603	3129	3131	3135	rVB	266858	274486	6.80%	0.773%
35	24.027	3536	3543	3551	rBV	1023820	2067110	51.23%	5.824%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042441.D
Acq On : 25 Oct 2023 17:12
Operator : MA/JU
Sample : 04941-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
72-12017

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-BM102123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

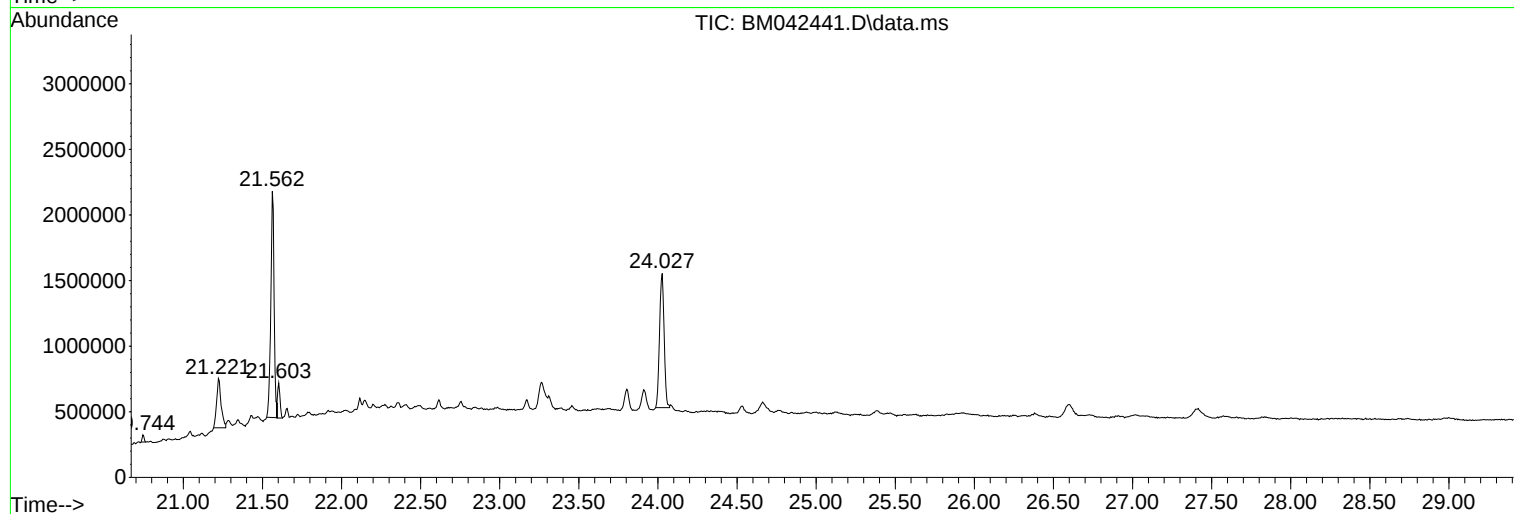
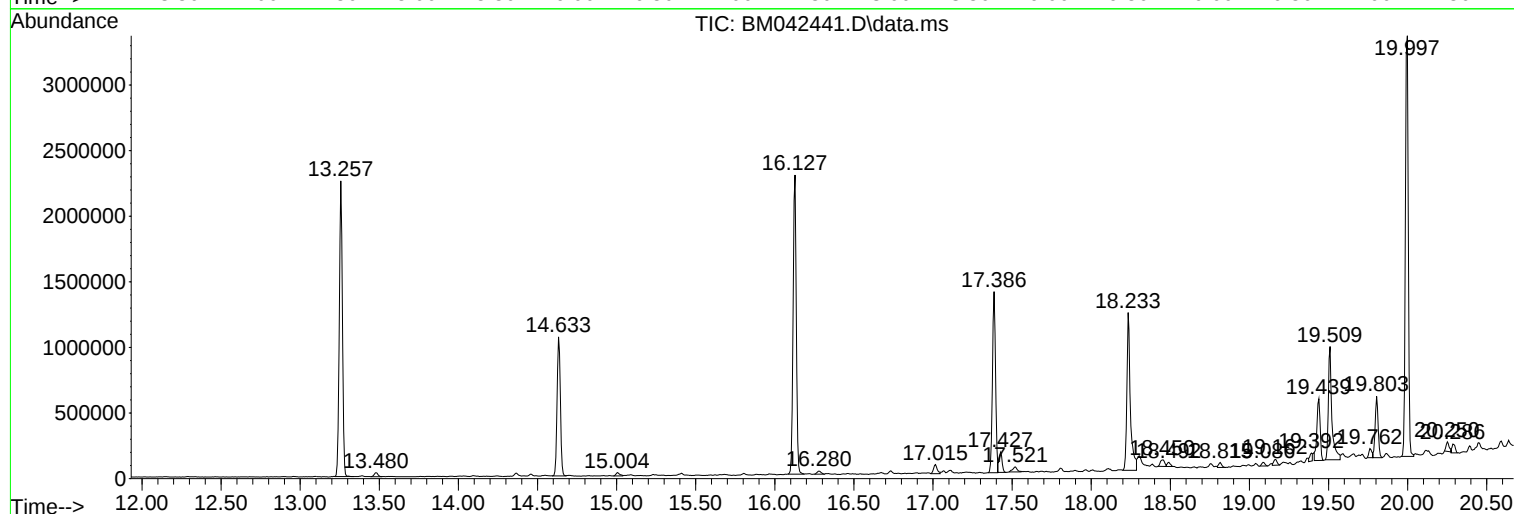
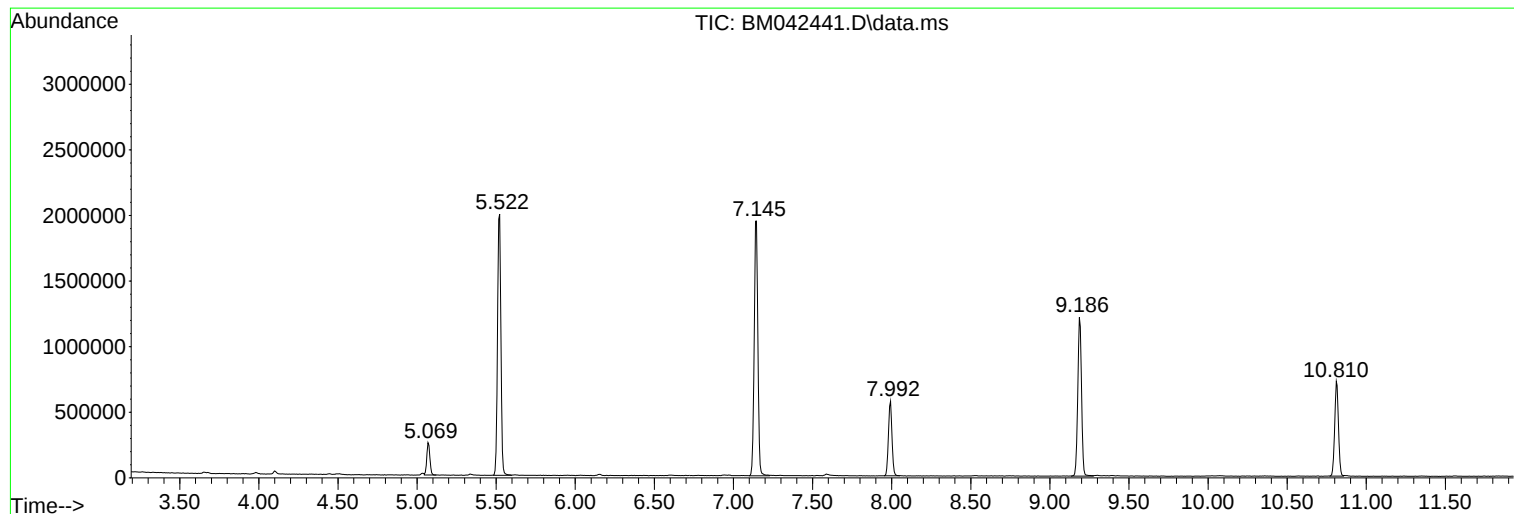
Sum of corrected areas: 35493217

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042441.D
Acq On : 25 Oct 2023 17:12
Operator : MA/JU
Sample : 04941-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
72-12017

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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\BM102523\
Data File : BM042441.D
Acq On : 25 Oct 2023 17:12
Operator : MA/JU
Sample : 04941-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
72-12017

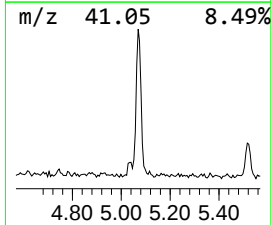
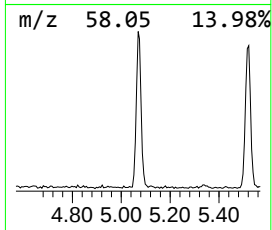
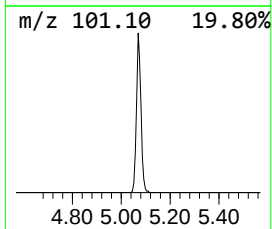
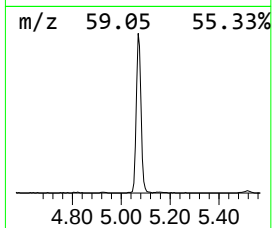
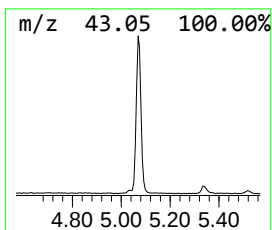
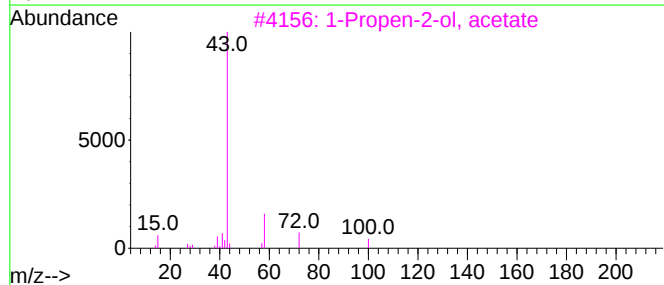
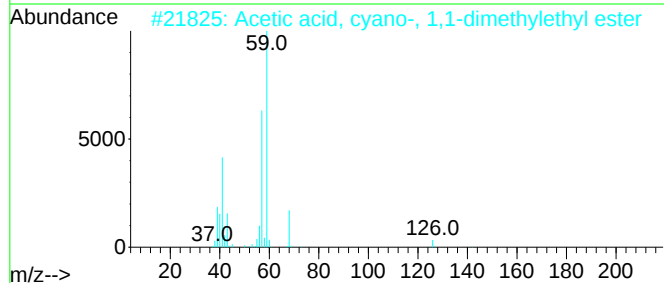
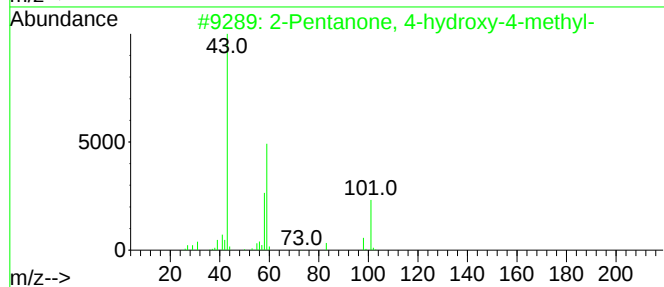
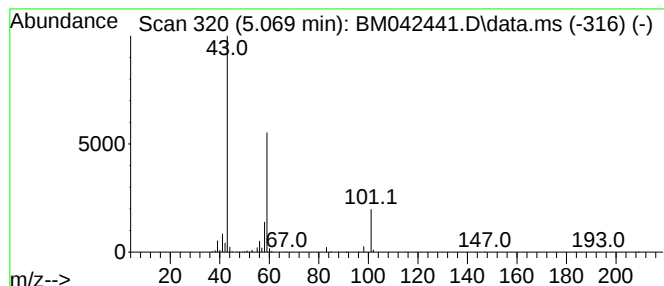
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	7.50 ng	334079	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042441.D
Acq On : 25 Oct 2023 17:12
Operator : MA/JU
Sample : 04941-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
72-12017

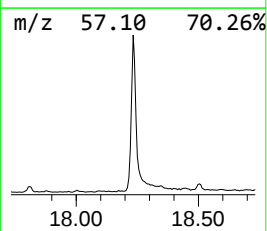
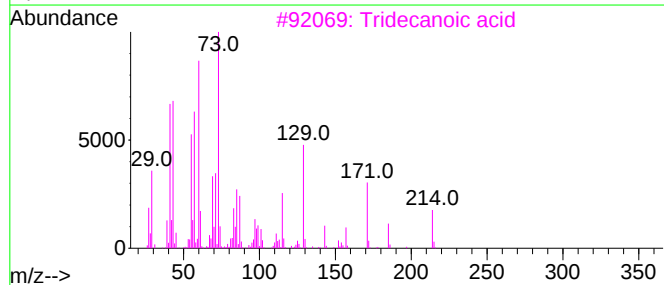
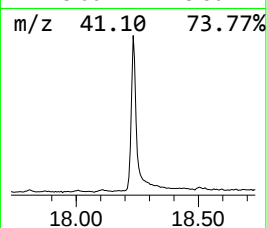
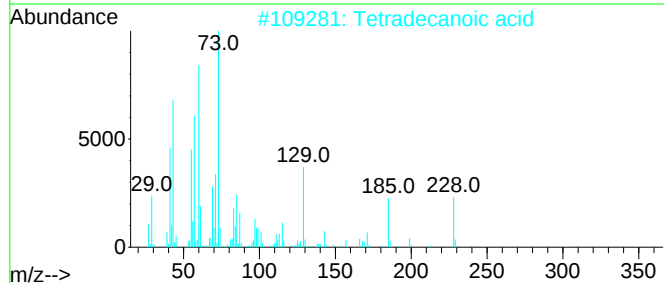
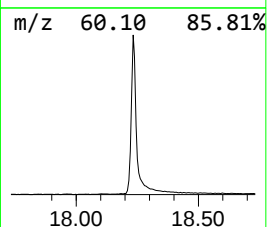
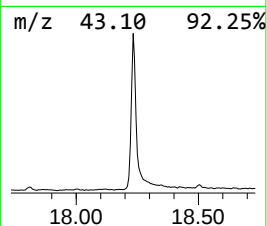
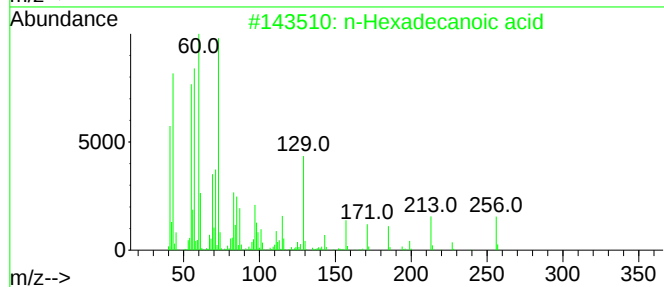
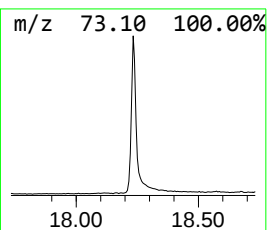
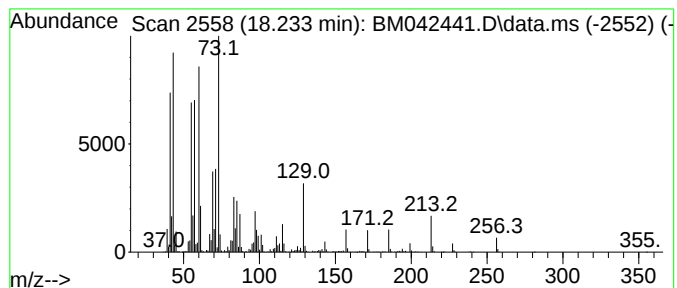
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.233	19.59 ng	1844150	Phenanthrene-d10	17.386

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	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042441.D
Acq On : 25 Oct 2023 17:12
Operator : MA/JU
Sample : 04941-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
72-12017

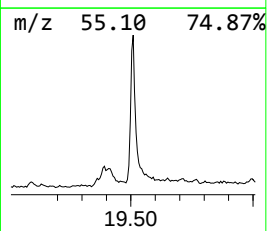
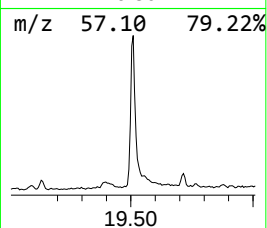
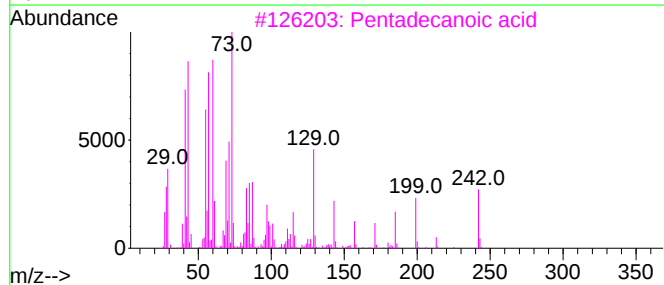
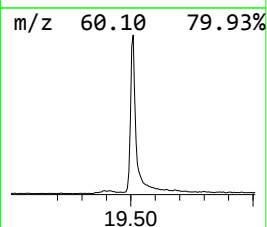
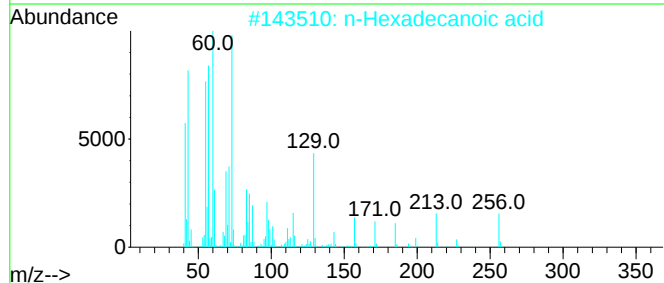
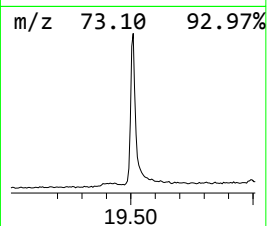
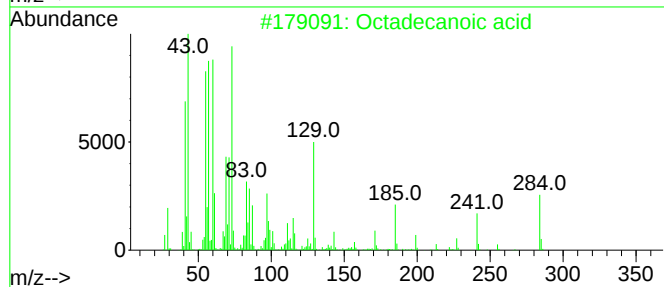
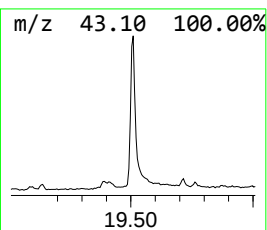
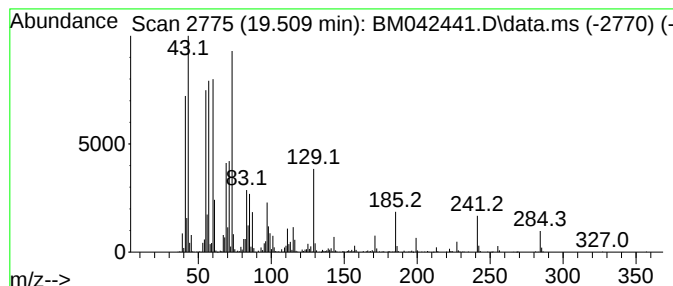
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.509	10.39 ng	1313280	Chrysene-d12	21.562

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	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042441.D
Acq On : 25 Oct 2023 17:12
Operator : MA/JU
Sample : 04941-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
72-12017

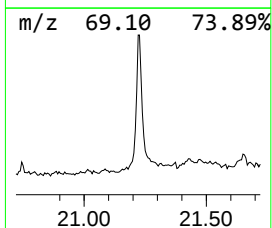
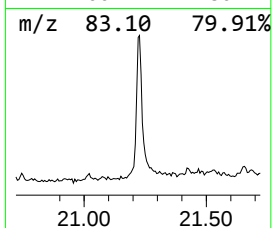
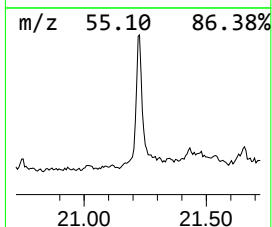
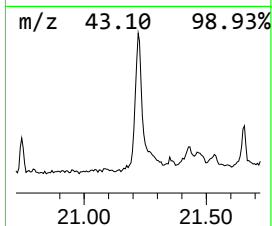
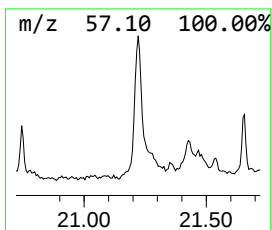
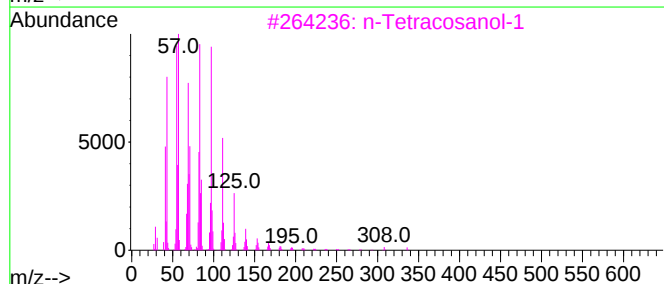
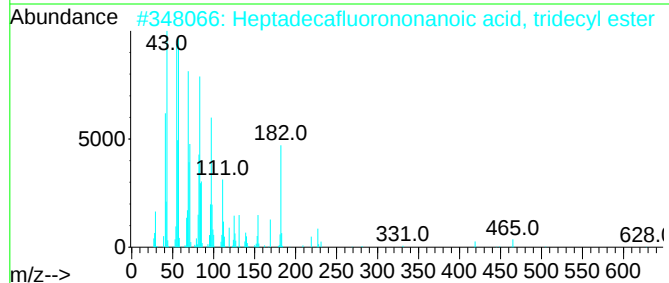
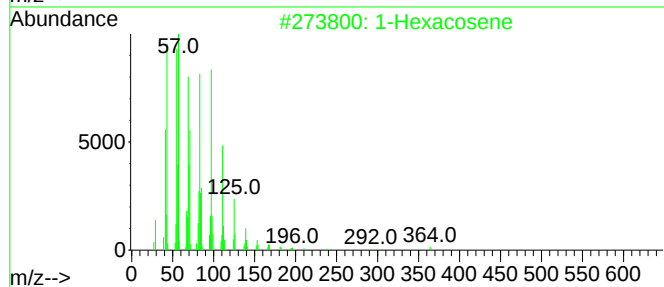
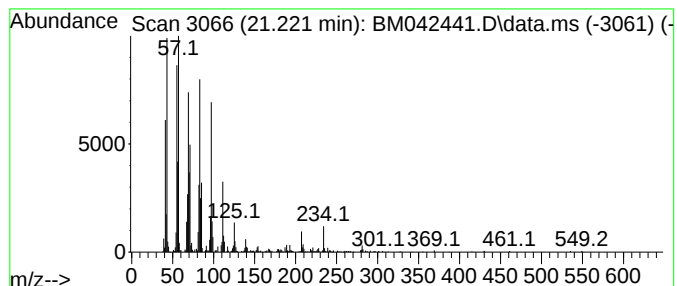
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.221	5.81 ng	733900	Chrysene-d12	21.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	94
2			Heptadecafluorononanoic acid, tr...	646	C22H27F17O2	1000356-02-9	91
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042441.D
Acq On : 25 Oct 2023 17:12
Operator : MA/JU
Sample : 04941-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
72-12017

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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
2-Pentanone, 4-...	5.069	7.5	ng	334079	1	7.992	890500	20.0
n-Hexadecanoic ...	18.233	19.6	ng	1844150	4	17.386	1882380	20.0
Octadecanoic acid	19.509	10.4	ng	1313280	5	21.562	2528200	20.0
1-Hexacosene	21.221	5.8	ng	733900	5	21.562	2528200	20.0