

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111022\
 Data File : BM037455.D
 Acq On : 10 Nov 2022 17:22
 Operator : CG/JU
 Sample : N5495-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-29A

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-BM102822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037455.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	307	312	319	rBV	482947	653766	6.76%	1.154%
2	5.387	385	391	407	rBV	3163355	4462279	46.12%	7.875%
3	6.992	656	664	676	rBV	2871789	4584776	47.39%	8.091%
4	7.810	795	803	810	rBV	831103	1258169	13.00%	2.220%
5	8.981	994	1002	1016	rBV	1779905	2920476	30.19%	5.154%
6	9.945	1150	1166	1194	rBV	562544	2102520	21.73%	3.711%
7	10.610	1272	1279	1292	rBV	1042948	1713657	17.71%	3.024%
8	13.074	1690	1698	1714	rBV	4643706	6473873	66.92%	11.425%
9	14.451	1925	1932	1950	rVB	1462467	2217071	22.92%	3.913%
10	15.939	2175	2185	2199	rBV	3852763	5445158	56.28%	9.610%
11	16.239	2231	2236	2244	rBV	132595	198814	2.06%	0.351%
12	16.598	2292	2297	2306	rBV2	86280	175795	1.82%	0.310%
13	16.851	2335	2340	2348	rBV	129479	200776	2.08%	0.354%
14	17.192	2392	2398	2403	rBV	1846128	2526797	26.12%	4.459%
15	18.027	2536	2540	2545	rBV	179869	284065	2.94%	0.501%
16	18.086	2545	2550	2560	rVV	1100129	1653922	17.10%	2.919%
17	18.380	2596	2600	2604	rBV3	83705	131406	1.36%	0.232%
18	18.427	2604	2608	2619	rVB3	105663	207352	2.14%	0.366%
19	19.003	2701	2706	2709	rBV2	141832	191260	1.98%	0.338%
20	19.250	2744	2748	2756	rVB	312364	460786	4.76%	0.813%
21	19.368	2763	2768	2779	rBV	668669	1125927	11.64%	1.987%
22	19.609	2806	2809	2818	rVB	319173	487784	5.04%	0.861%
23	19.815	2839	2844	2849	rBV	8837836	9674596	100.00%	17.074%
24	20.092	2888	2891	2899	rVB4	156743	255089	2.64%	0.450%
25	20.509	2959	2962	2966	rBV	308682	352067	3.64%	0.621%
26	21.080	3056	3059	3067	rVB2	655995	886449	9.16%	1.564%
27	21.374	3104	3109	3113	rBV	2457822	3178233	32.85%	5.609%
28	23.703	3500	3505	3512	rVB2	1629457	2840998	29.37%	5.014%

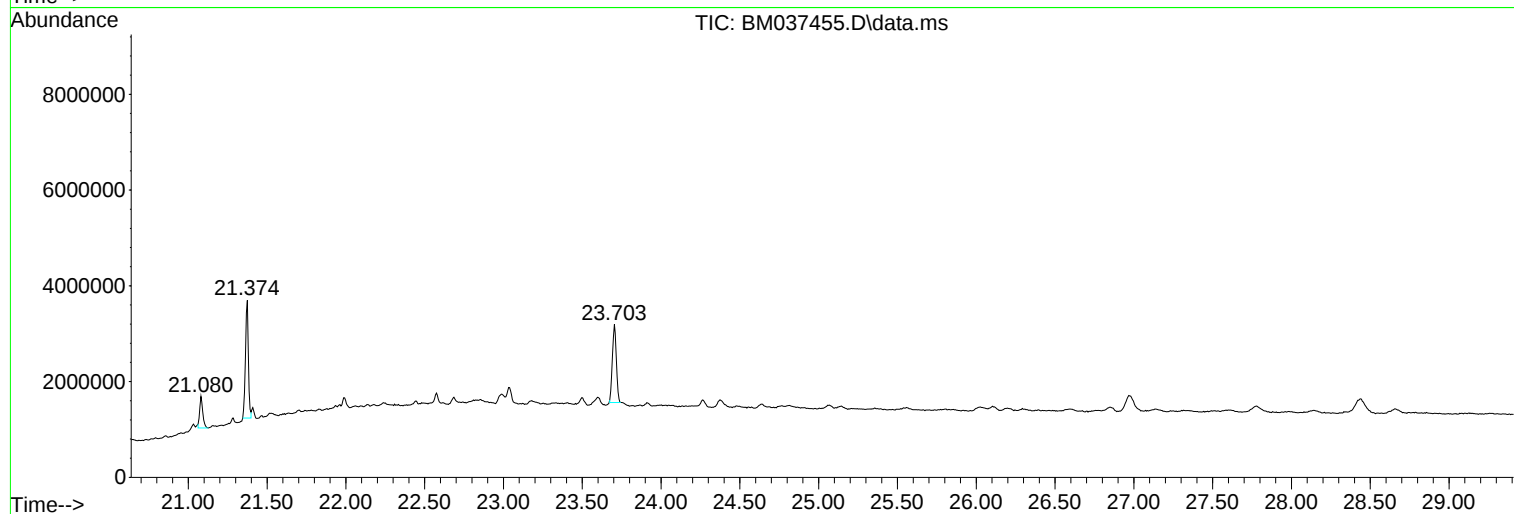
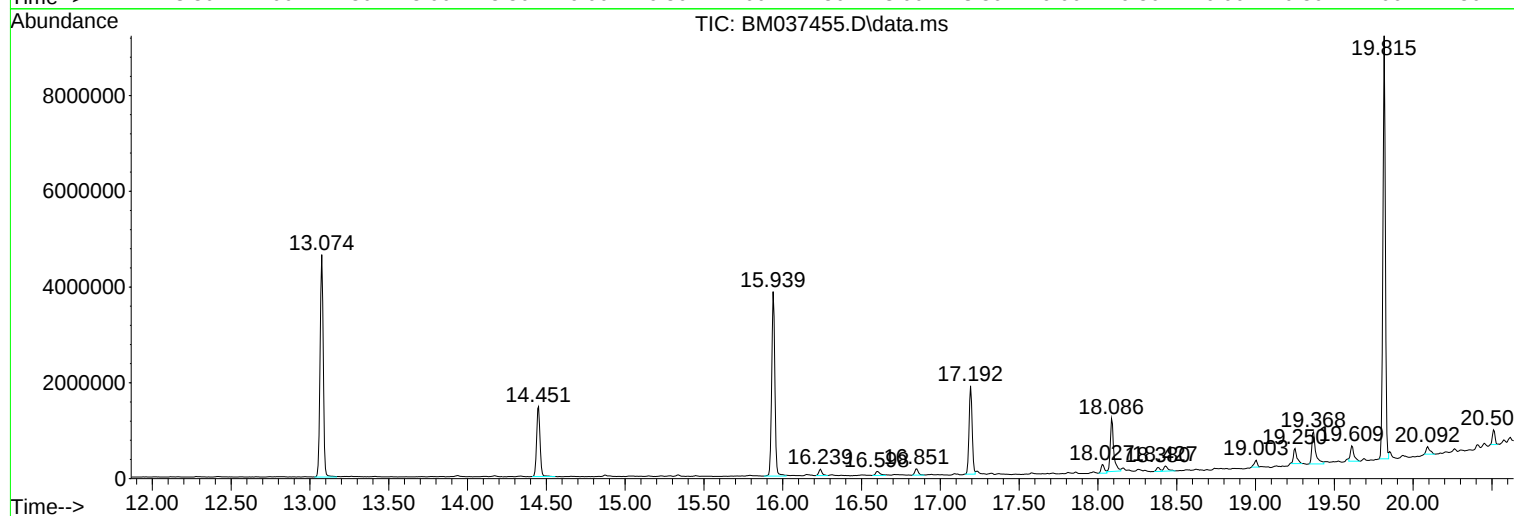
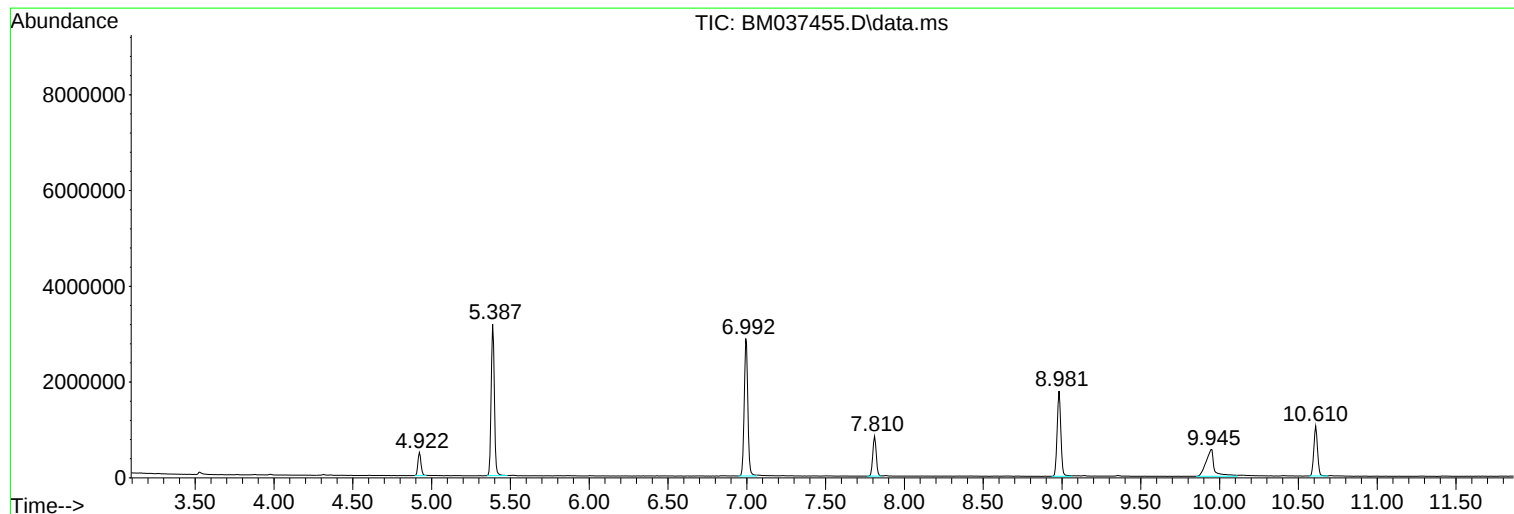
Sum of corrected areas: 56663861

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111022\
Data File : BM037455.D
Acq On : 10 Nov 2022 17:22
Operator : CG/JU
Sample : N5495-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-29A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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\BM111022\
Data File : BM037455.D
Acq On : 10 Nov 2022 17:22
Operator : CG/JU
Sample : N5495-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-29A

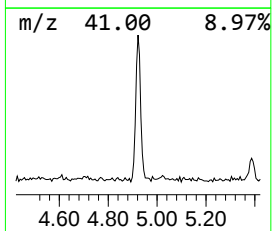
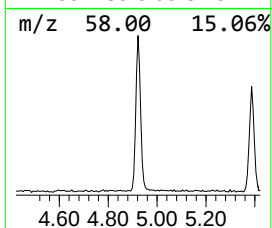
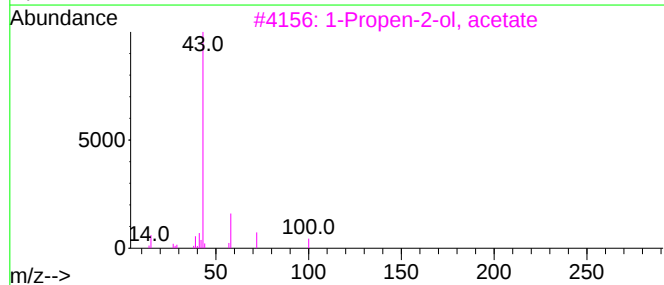
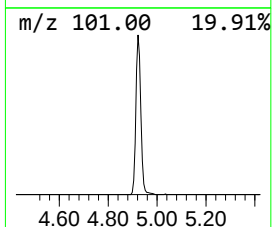
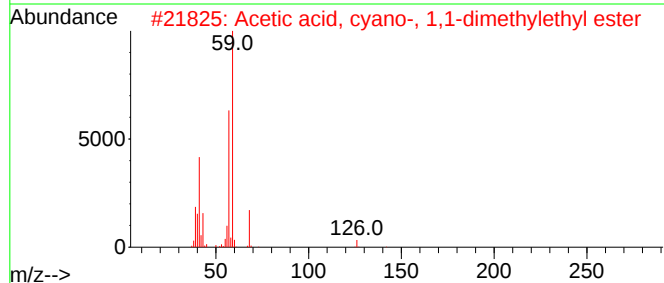
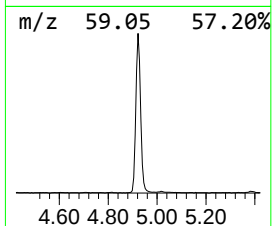
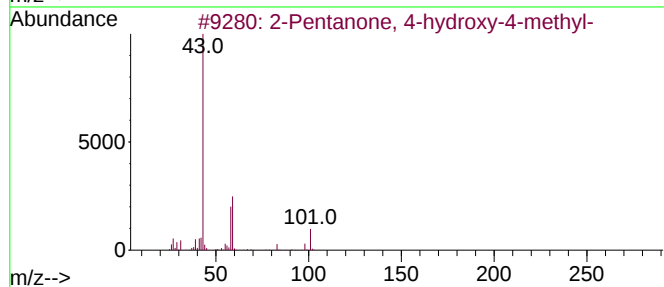
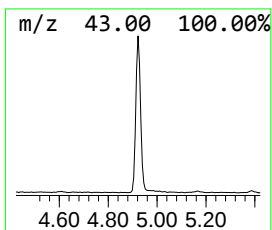
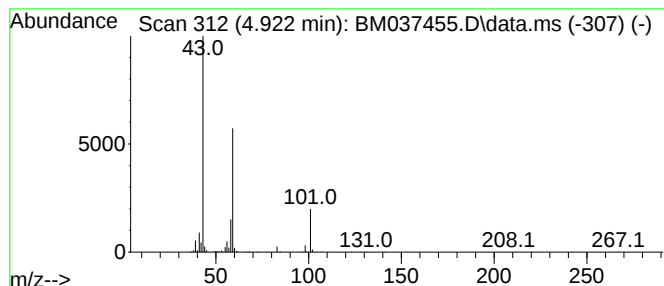
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	10.39 ng	653766	1,4-Dichlorobenzene-d4	7.810

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	17		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111022\
Data File : BM037455.D
Acq On : 10 Nov 2022 17:22
Operator : CG/JU
Sample : N5495-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

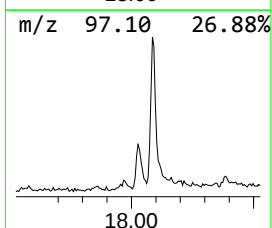
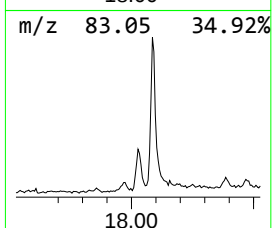
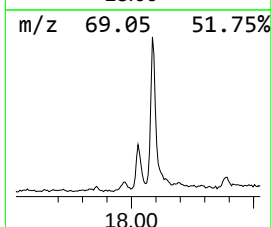
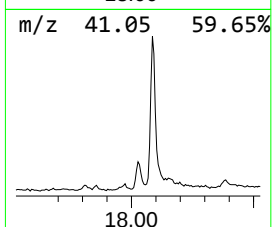
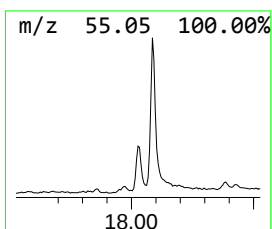
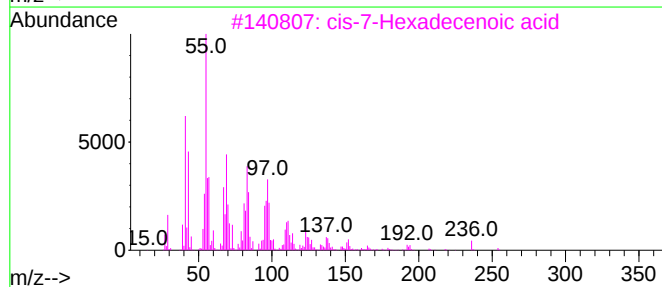
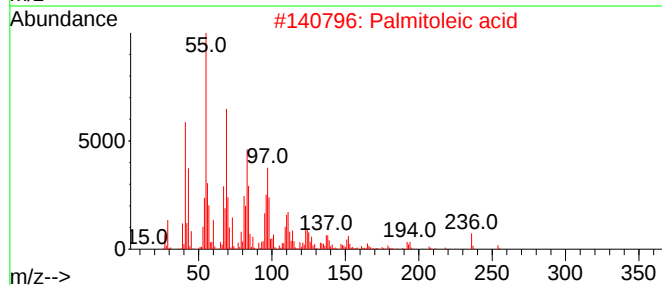
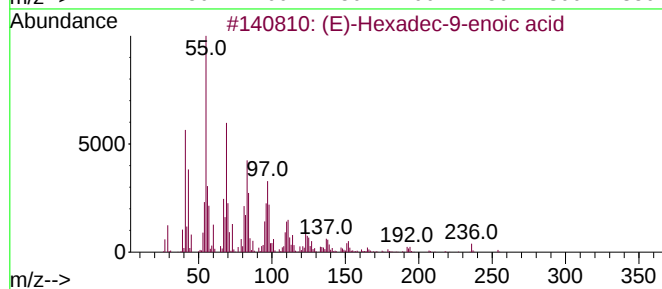
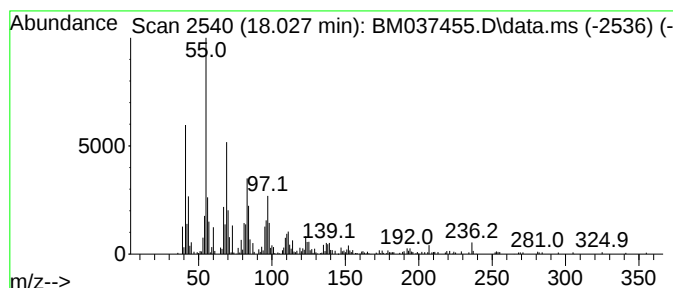
Instrument :
BNA_M
ClientSampleId :
SB-29A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 (E)-Hexadec-9-enoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.027	2.25 ng	284065	Phenanthrene-d10	17.192	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	99
2	Palmitoleic acid	254	C16H30O2	000373-49-9	99
3	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	99
4	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	98
5	6-Pentadecenoic acid, 13-methyl-...	254	C16H30O2	682751-34-4	92



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111022\
Data File : BM037455.D
Acq On : 10 Nov 2022 17:22
Operator : CG/JU
Sample : N5495-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

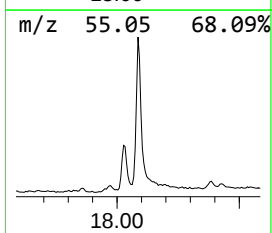
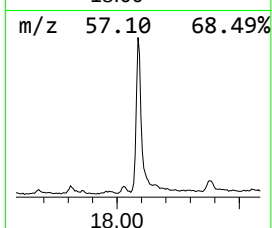
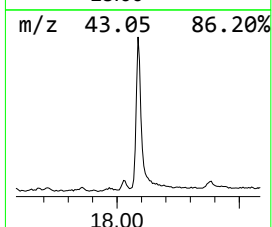
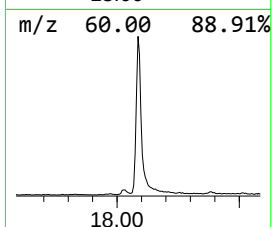
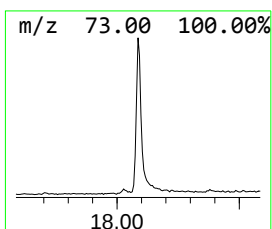
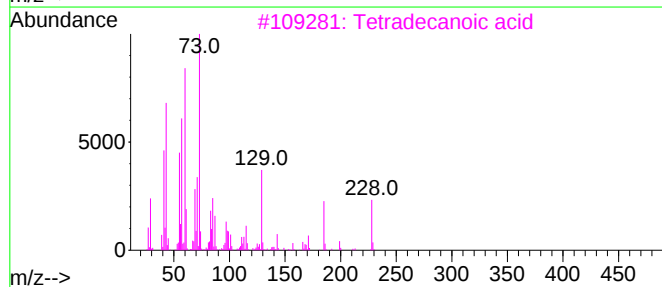
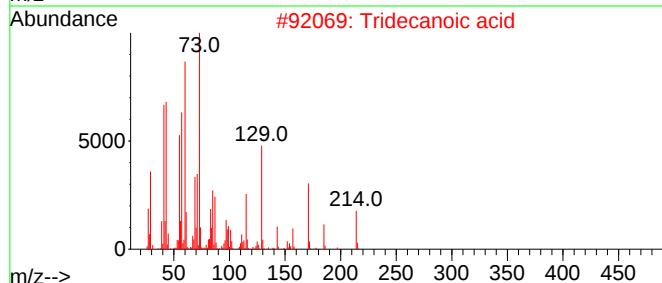
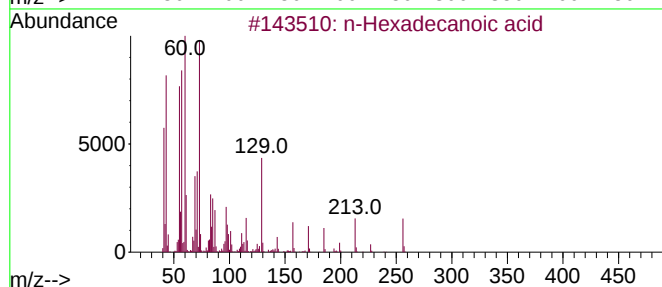
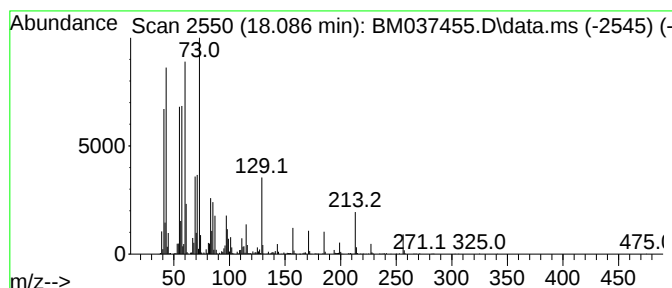
Instrument :
BNA_M
ClientSampleId :
SB-29A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.086	13.09 ng	1653920	Phenanthrene-d10	17.192	
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	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111022\
Data File : BM037455.D
Acq On : 10 Nov 2022 17:22
Operator : CG/JU
Sample : N5495-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-29A

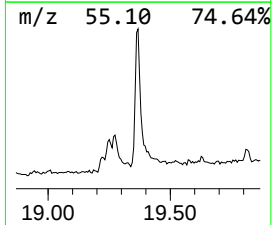
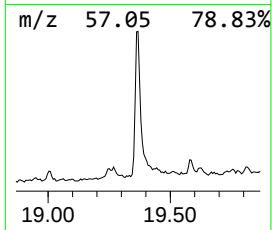
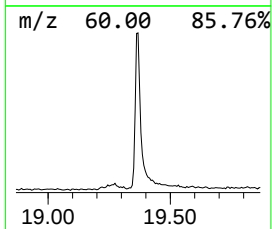
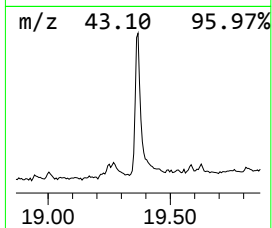
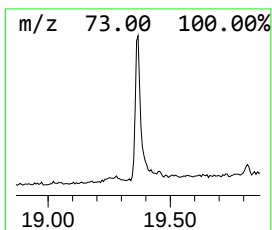
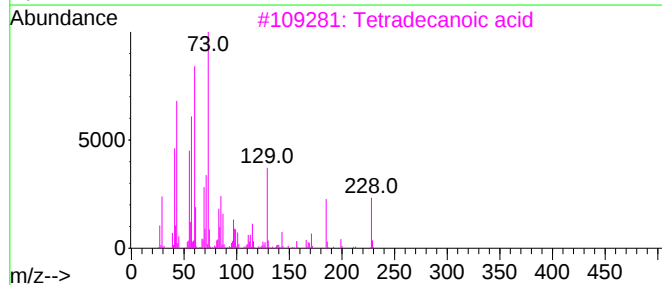
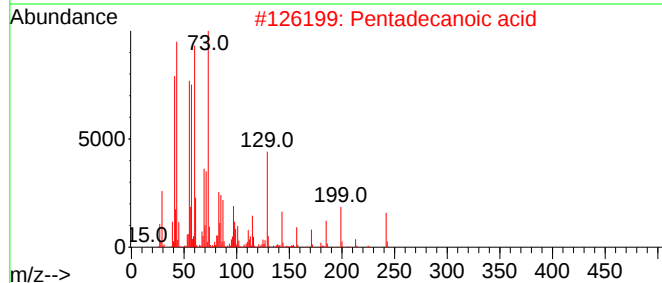
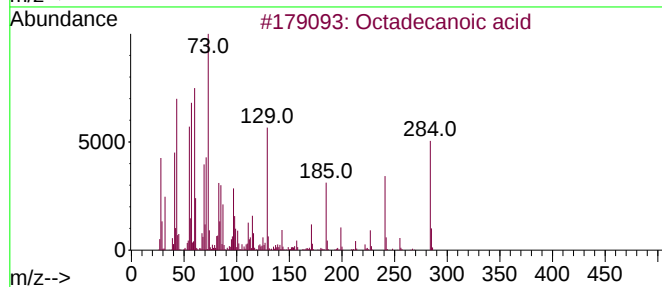
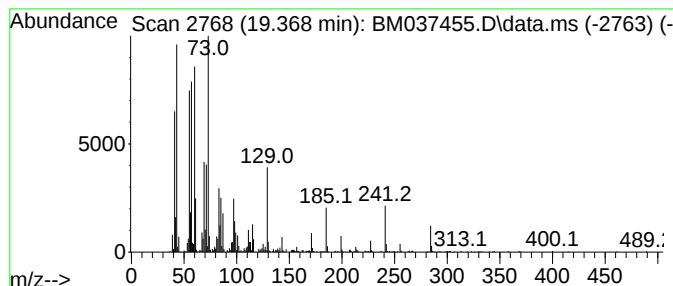
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.368	7.09 ng	1125930	Chrysene-d12	21.374

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	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111022\
Data File : BM037455.D
Acq On : 10 Nov 2022 17:22
Operator : CG/JU
Sample : N5495-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

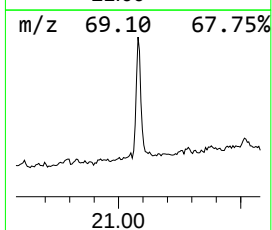
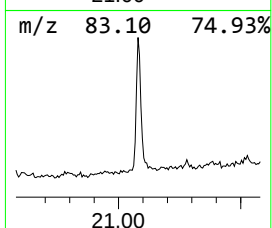
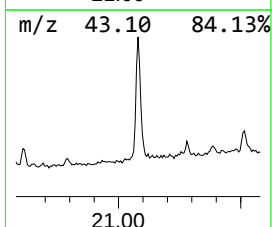
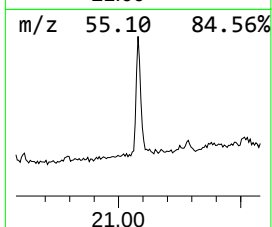
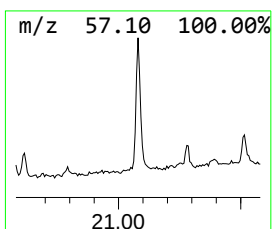
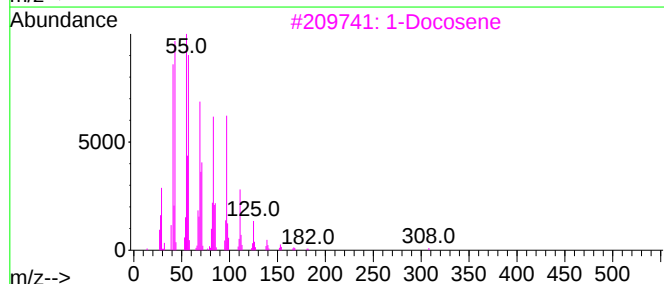
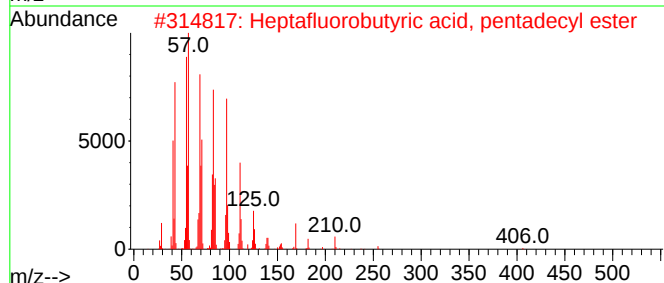
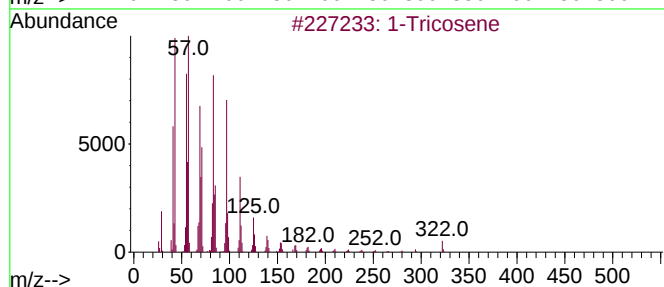
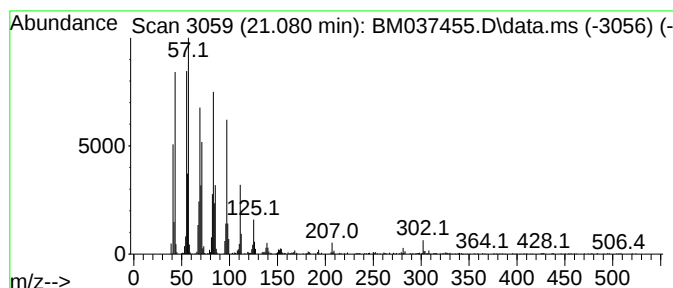
Instrument :
BNA_M
ClientSampleId :
SB-29A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.080	5.58 ng	886449	Chrysene-d12	21.374	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	1-Docosene	308	C22H44	001599-67-3	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	1-Hexacosene	364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111022\
Data File : BM037455.D
Acq On : 10 Nov 2022 17:22
Operator : CG/JU
Sample : N5495-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-29A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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-...	4.922	10.4	ng	653766	1	7.810	1258170	20.0
(E)-Hexadec-9-e...	18.027	2.3	ng	284065	4	17.192	2526800	20.0
n-Hexadecanoic ...	18.086	13.1	ng	1653920	4	17.192	2526800	20.0
Octadecanoic acid	19.368	7.1	ng	1125930	5	21.374	3178230	20.0
1-Tricosene	21.080	5.6	ng	886449	5	21.374	3178230	20.0