

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081523\
 Data File : BM041406.D
 Acq On : 15 Aug 2023 15:13
 Operator : MA/JU
 Sample : 04006-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 E-1

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: BM041406.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.340	360	366	384	rBV	1219577	1763383	40.97%	5.058%
2	6.945	633	639	660	rBV	1159450	1897731	44.09%	5.443%
3	7.763	772	778	788	rBV	540004	835527	19.41%	2.396%
4	8.939	970	978	996	rBV	568871	998573	23.20%	2.864%
5	10.569	1247	1255	1272	rBV	642097	1100378	25.57%	3.156%
6	13.045	1669	1676	1687	rBV	1456367	2110994	49.05%	6.055%
7	14.427	1905	1911	1921	rBV	970265	1343098	31.21%	3.852%
8	14.857	1979	1984	1992	rBV	73781	143327	3.33%	0.411%
9	15.927	2160	2166	2175	rBV	1460556	2041803	47.44%	5.856%
10	16.592	2274	2279	2288	rBV3	43991	84555	1.96%	0.243%
11	17.186	2371	2380	2397	rBV	1140568	1692590	39.33%	4.855%
12	17.962	2508	2512	2517	rBV6	23849	44973	1.04%	0.129%
13	18.098	2527	2535	2563	rBV	2538503	4304029	100.00%	12.345%
14	18.639	2623	2627	2635	rBV4	29719	55235	1.28%	0.158%
15	19.192	2712	2721	2730	rBV	843896	2046882	47.56%	5.871%
16	19.374	2747	2752	2772	rBV	1566976	2419801	56.22%	6.941%
17	19.762	2815	2818	2823	rVB	32993	54700	1.27%	0.157%
18	19.827	2824	2829	2837	rBV	3042278	3521355	81.82%	10.100%
19	20.521	2941	2947	2953	rBV	443712	604535	14.05%	1.734%
20	20.968	3018	3023	3030	rBV2	182641	342262	7.95%	0.982%
21	21.097	3041	3045	3049	rBV	228992	324252	7.53%	0.930%
22	21.303	3075	3080	3086	rVB	806152	910591	21.16%	2.612%
23	21.397	3091	3096	3099	rBV	1617177	2115873	49.16%	6.069%
24	21.433	3099	3102	3111	rVB2	432065	907847	21.09%	2.604%
25	22.609	3298	3302	3316	rVB2	377276	656029	15.24%	1.882%
26	23.756	3491	3497	3512	rVB	1296211	2544603	59.12%	7.298%

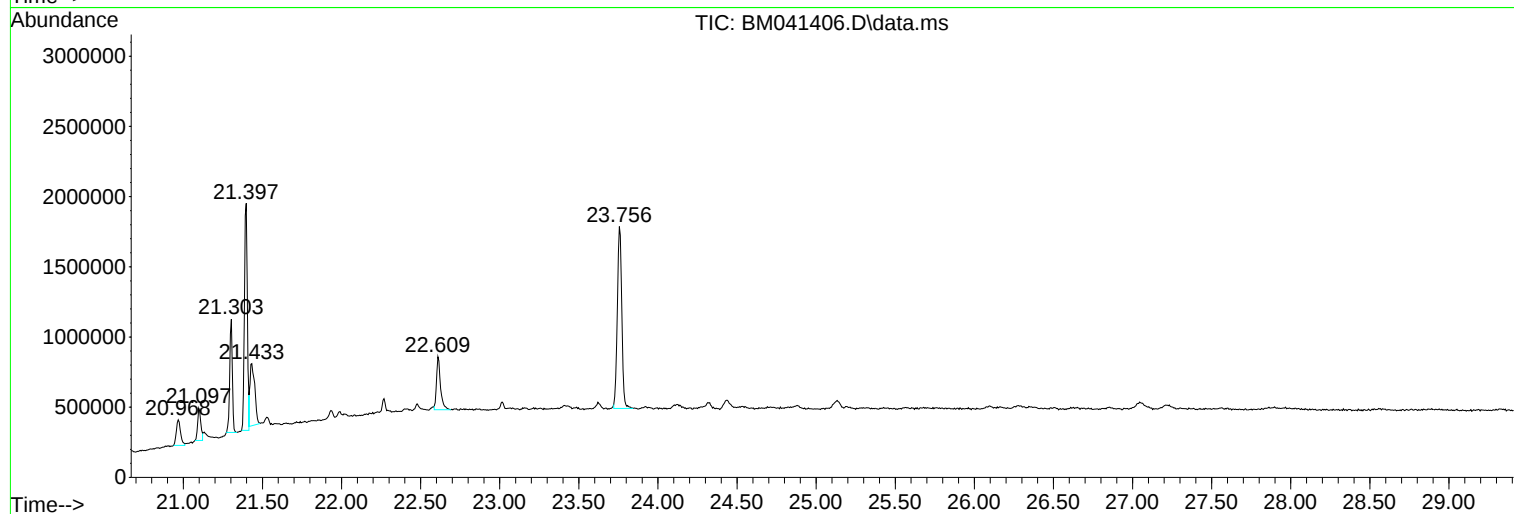
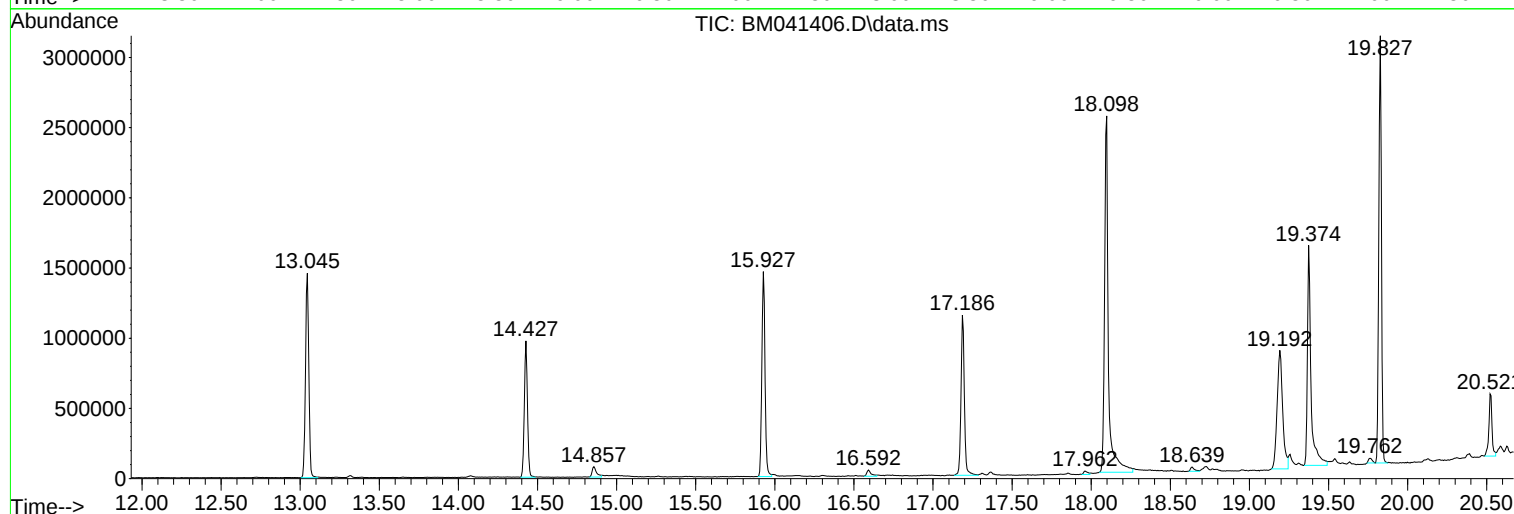
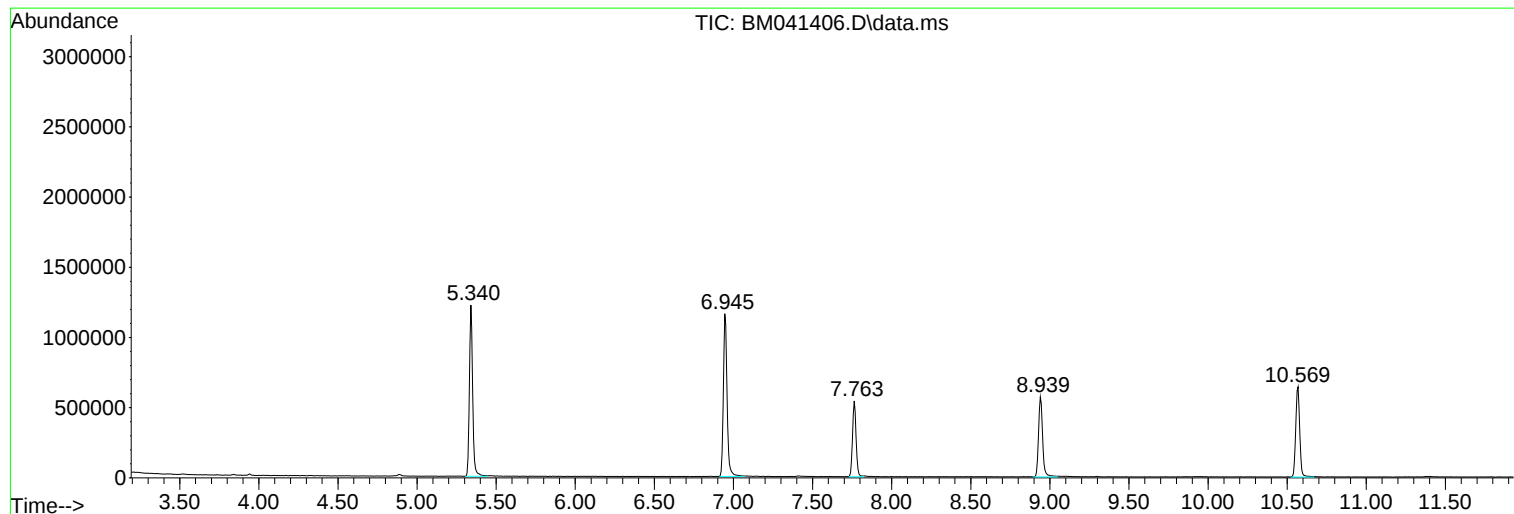
Sum of corrected areas: 34864926

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081523\
Data File : BM041406.D
Acq On : 15 Aug 2023 15:13
Operator : MA/JU
Sample : 04006-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E-1

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\BM081523\
Data File : BM041406.D
Acq On : 15 Aug 2023 15:13
Operator : MA/JU
Sample : 04006-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E-1

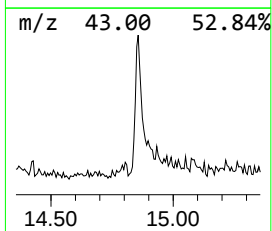
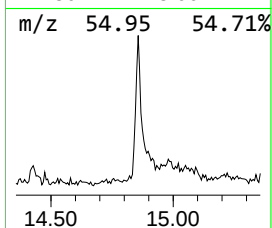
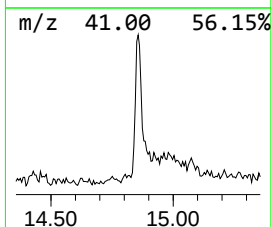
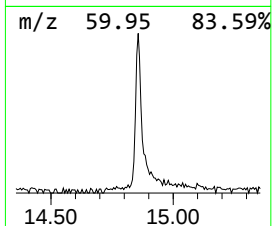
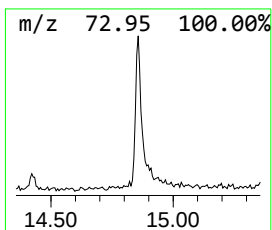
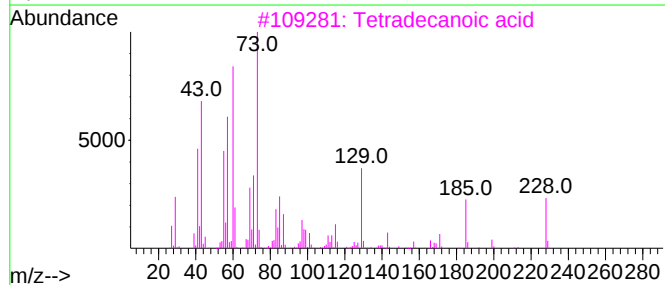
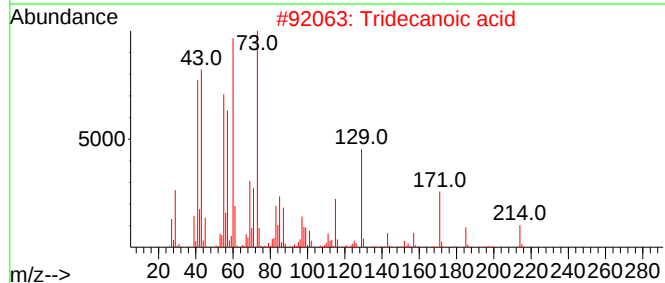
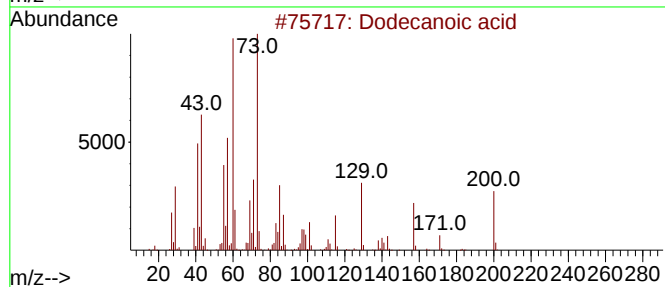
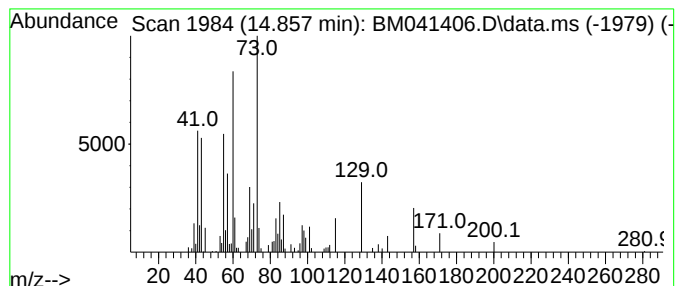
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	2.13 ng	143327	Acenaphthene-d10	14.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Nonanoic acid	158	C9H18O2	000112-05-0	53
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081523\
Data File : BM041406.D
Acq On : 15 Aug 2023 15:13
Operator : MA/JU
Sample : 04006-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E-1

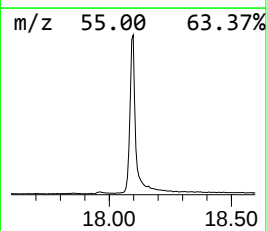
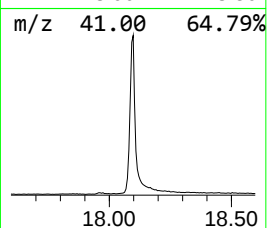
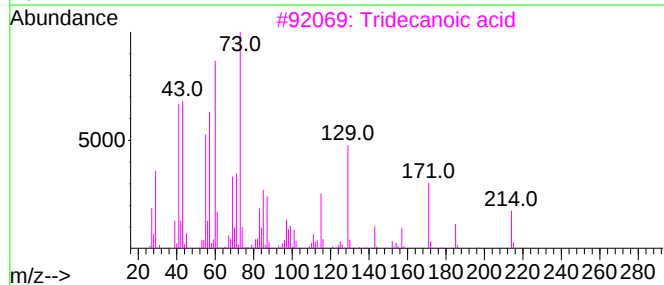
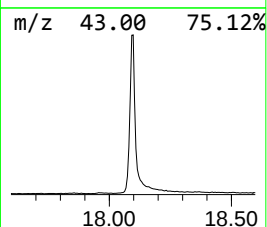
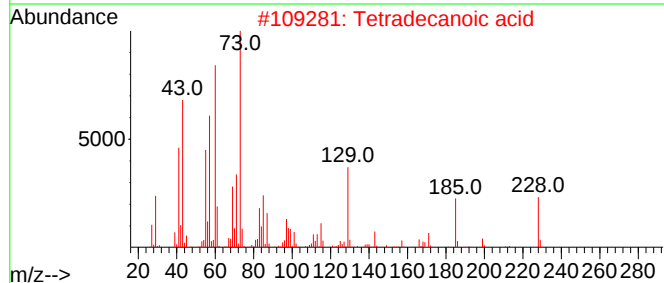
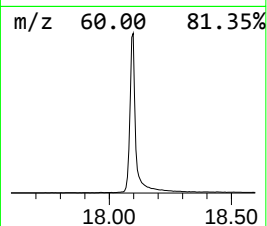
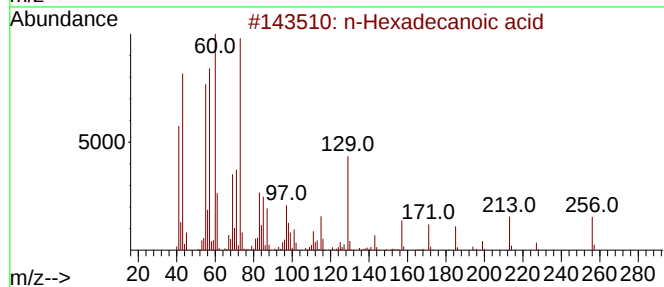
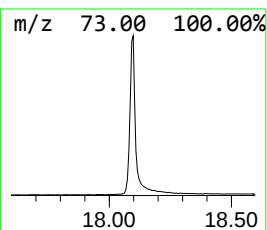
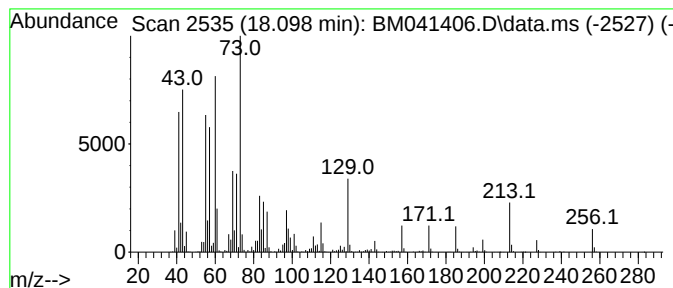
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.098	50.86 ng	4304030	Phenanthrene-d10	17.186

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	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081523\
Data File : BM041406.D
Acq On : 15 Aug 2023 15:13
Operator : MA/JU
Sample : 04006-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E-1

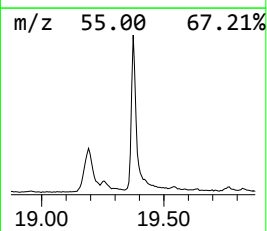
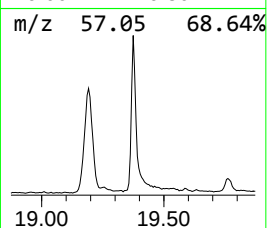
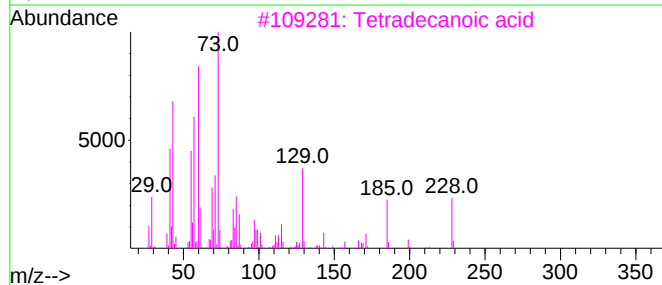
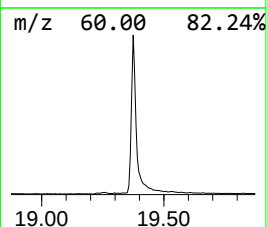
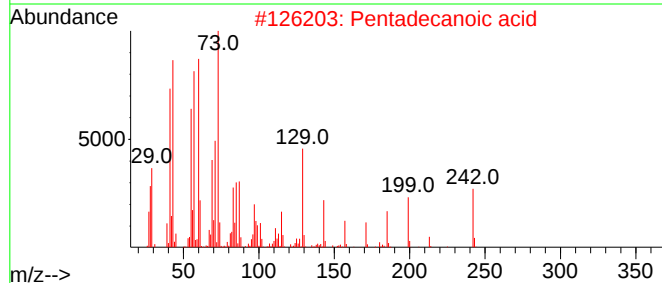
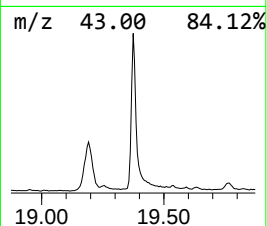
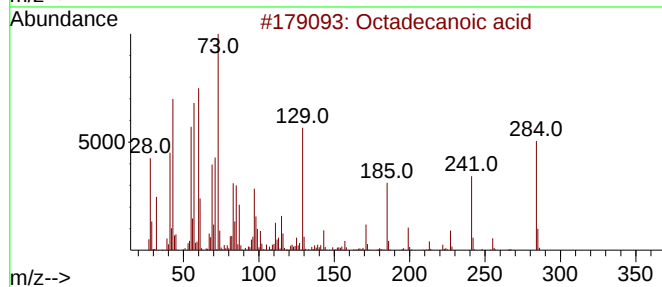
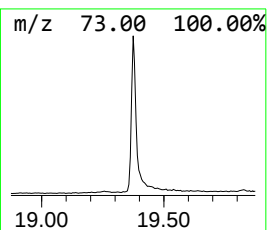
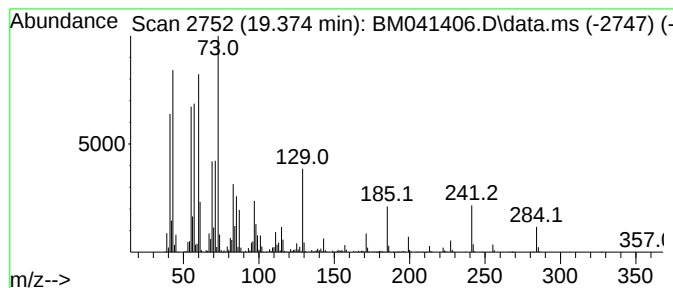
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.374	22.87 ng	2419800	Chrysene-d12	21.397

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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081523\
Data File : BM041406.D
Acq On : 15 Aug 2023 15:13
Operator : MA/JU
Sample : 04006-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E-1

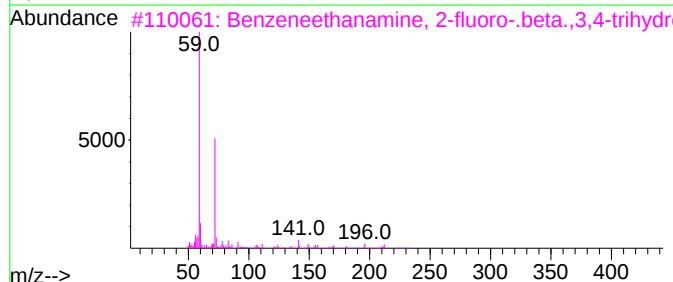
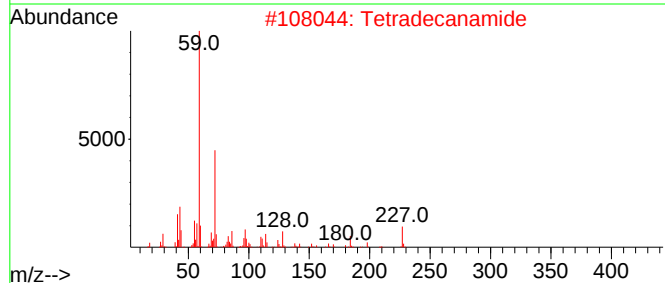
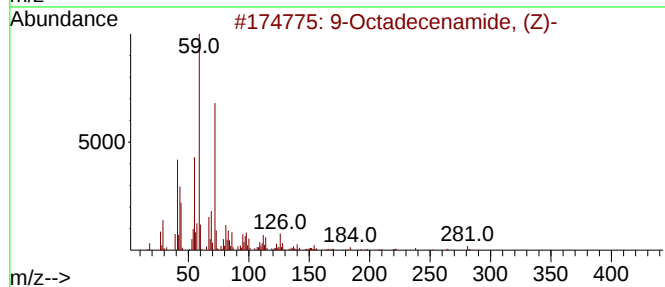
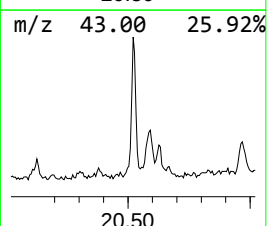
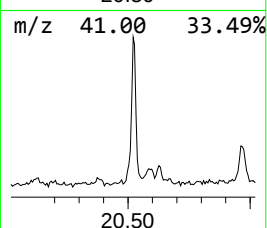
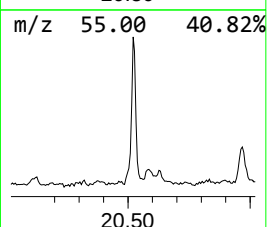
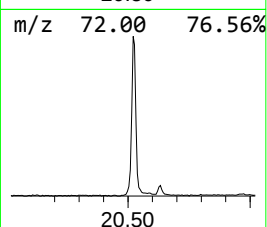
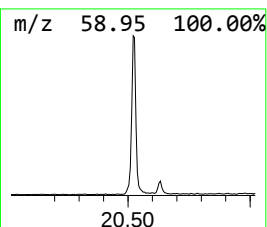
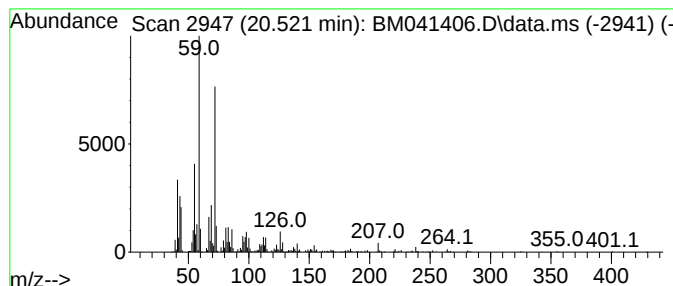
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.521	5.71 ng	604535	Chrysene-d12	21.397

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2			Tetradecanamide	227	C14H29NO	000638-58-4	72
3			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
4			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59
5			3-Cyclohexylpropionamide	155	C9H17NO	004361-29-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081523\
Data File : BM041406.D
Acq On : 15 Aug 2023 15:13
Operator : MA/JU
Sample : 04006-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

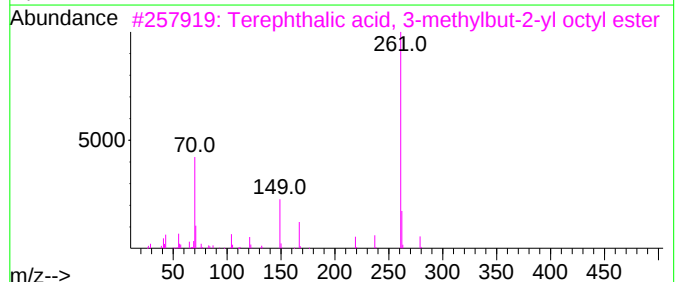
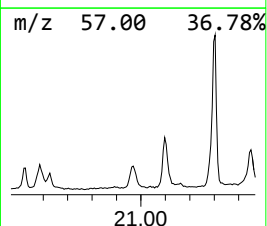
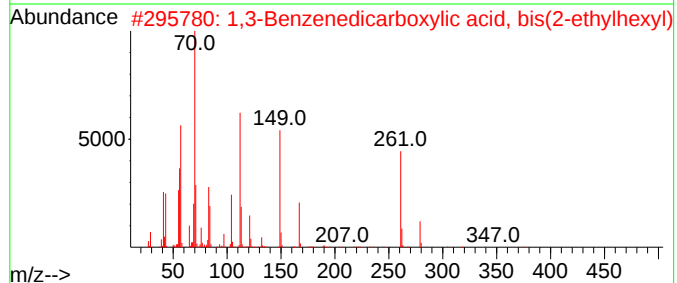
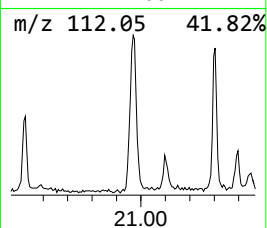
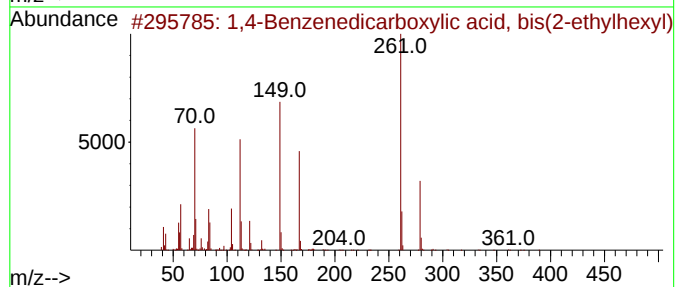
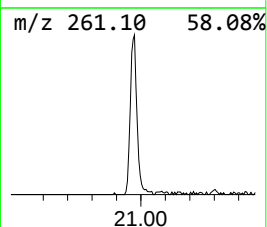
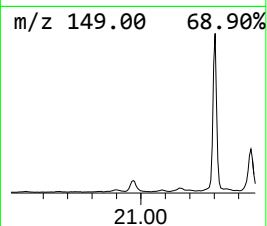
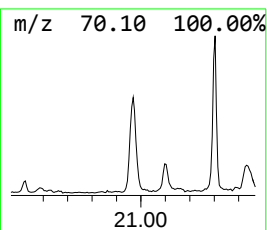
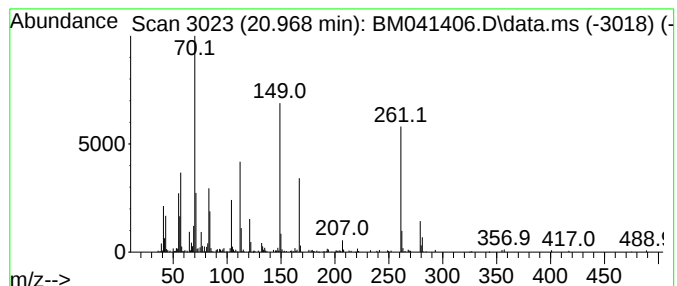
Instrument :
BNA_M
ClientSampleId :
E-1

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 6 1,4-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.968	3.24 ng	342262	Chrysene-d12	21.397	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	81
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	72
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	49
4	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	47
5	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081523\
Data File : BM041406.D
Acq On : 15 Aug 2023 15:13
Operator : MA/JU
Sample : 04006-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

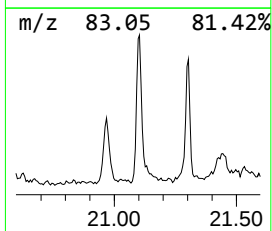
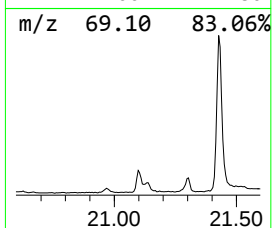
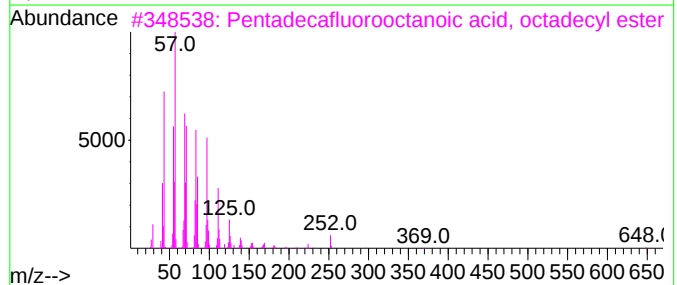
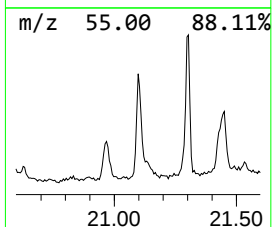
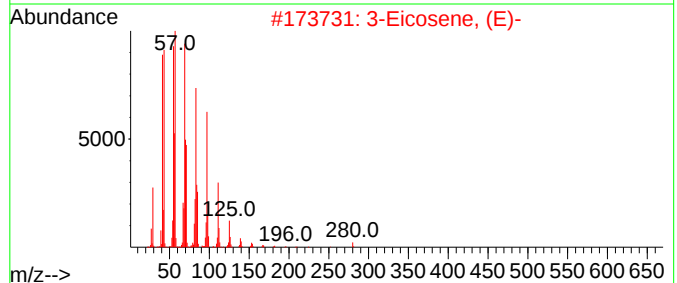
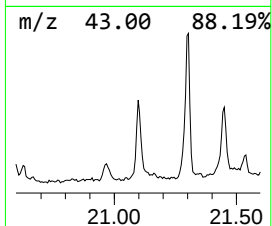
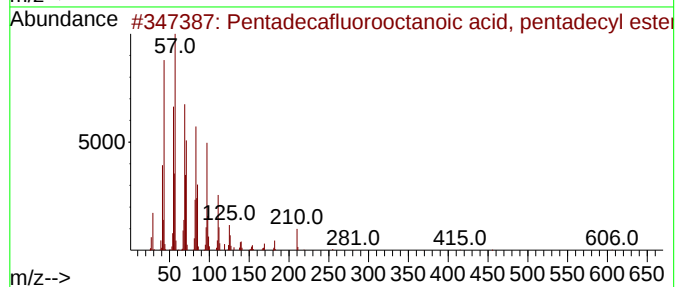
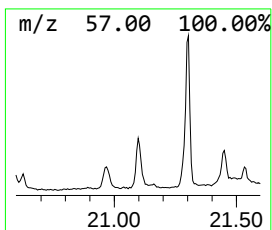
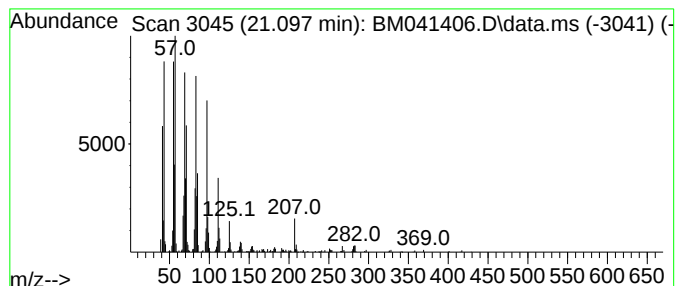
Instrument :
BNA_M
ClientSampleId :
E-1

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 7 Pentadecafluorooctanoic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.097	3.06 ng	324252	Chrysene-d12	21.397	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	92
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081523\
Data File : BM041406.D
Acq On : 15 Aug 2023 15:13
Operator : MA/JU
Sample : 04006-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E-1

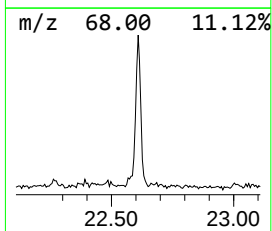
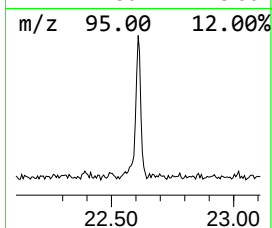
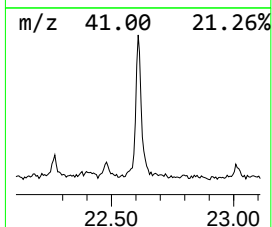
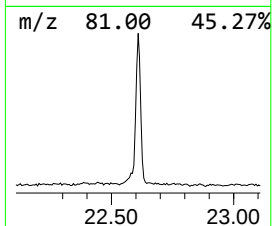
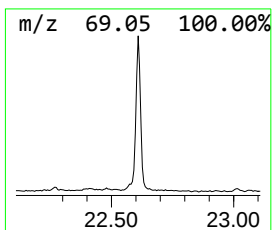
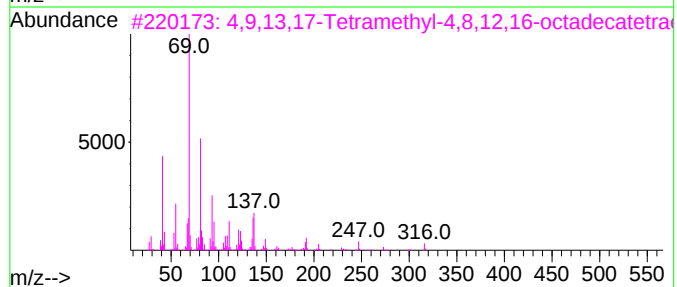
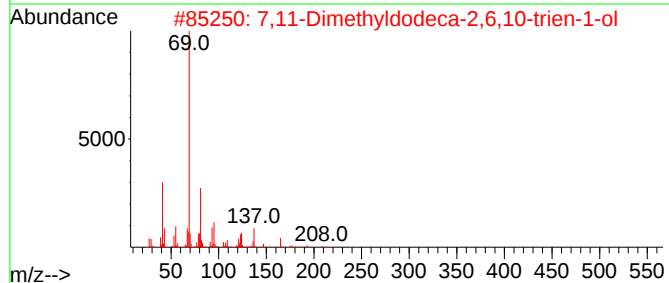
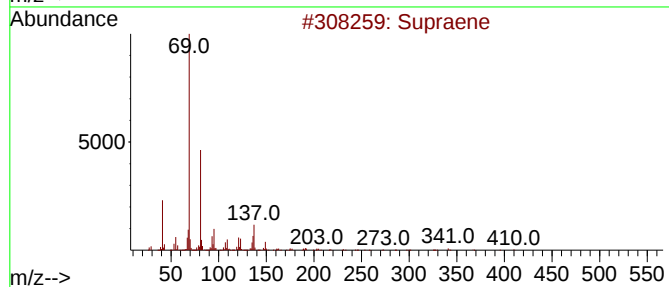
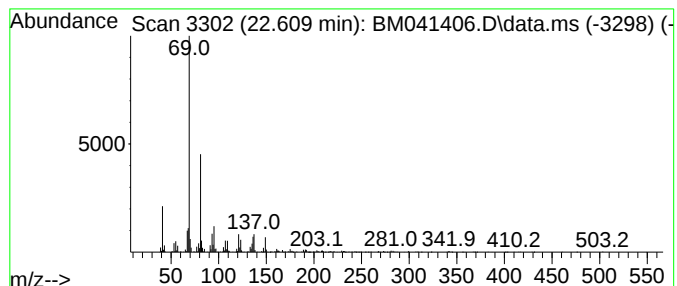
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.609	5.16 ng	656029	Perylene-d12	23.756

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4			Squalene	410	C30H50	000111-02-4	80
5			1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081523\
Data File : BM041406.D
Acq On : 15 Aug 2023 15:13
Operator : MA/JU
Sample : 04006-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E-1

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
Dodecanoic acid	14.857	2.1	ng	143327	3	14.427	1343100	20.0
n-Hexadecanoic ...	18.098	50.9	ng	4304030	4	17.186	1692590	20.0
Octadecanoic acid	19.374	22.9	ng	2419800	5	21.397	2115870	20.0
9-Octadecenamid...	20.521	5.7	ng	604535	5	21.397	2115870	20.0
1,4-Benzenedica...	20.968	3.2	ng	342262	5	21.397	2115870	20.0
Pentadecafluoro...	21.097	3.1	ng	324252	5	21.397	2115870	20.0
Supraene	22.609	5.2	ng	656029	6	23.756	2544600	20.0