

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
 Data File : BP013845.D
 Acq On : 17 Feb 2023 15:05
 Operator : CG/JU
 Sample : 01553-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TWP-01

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_P\Methods\8270E-BP021623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013845.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.175	332	338	351	rBV	413241	580427	4.90%	1.209%
2	5.646	411	418	432	rBV	1407287	2151426	18.18%	4.481%
3	7.252	684	691	706	rVB	883092	1395888	11.79%	2.907%
4	8.105	830	836	843	rBV	487936	785664	6.64%	1.636%
5	9.281	1027	1036	1050	rBV	1893295	3136664	26.50%	6.533%
6	10.169	1171	1187	1196	rBV	136362	325764	2.75%	0.678%
7	10.934	1309	1317	1329	rBV	611523	1055894	8.92%	2.199%
8	13.369	1723	1731	1741	rBV	5228202	7601640	64.23%	15.832%
9	14.740	1958	1964	1973	rBV	958376	1476479	12.47%	3.075%
10	15.551	2096	2102	2112	rVB	276343	390345	3.30%	0.813%
11	16.228	2211	2217	2234	rBV	4008593	5879991	49.68%	12.246%
12	17.492	2426	2432	2447	rBV	1251416	1894880	16.01%	3.946%
13	18.351	2573	2578	2586	rBV	423014	607266	5.13%	1.265%
14	19.575	2782	2786	2794	rBV	262677	392593	3.32%	0.818%
15	20.028	2858	2863	2869	rBV	9225799	11835671	100.00%	24.650%
16	21.251	3067	3071	3077	rBV	297546	458537	3.87%	0.955%
17	21.575	3121	3126	3131	rBV	1719667	2316100	19.57%	4.824%
18	21.692	3141	3146	3172	rBV	1900759	3196704	27.01%	6.658%
19	24.127	3554	3560	3573	rVB2	1191425	2533100	21.40%	5.276%

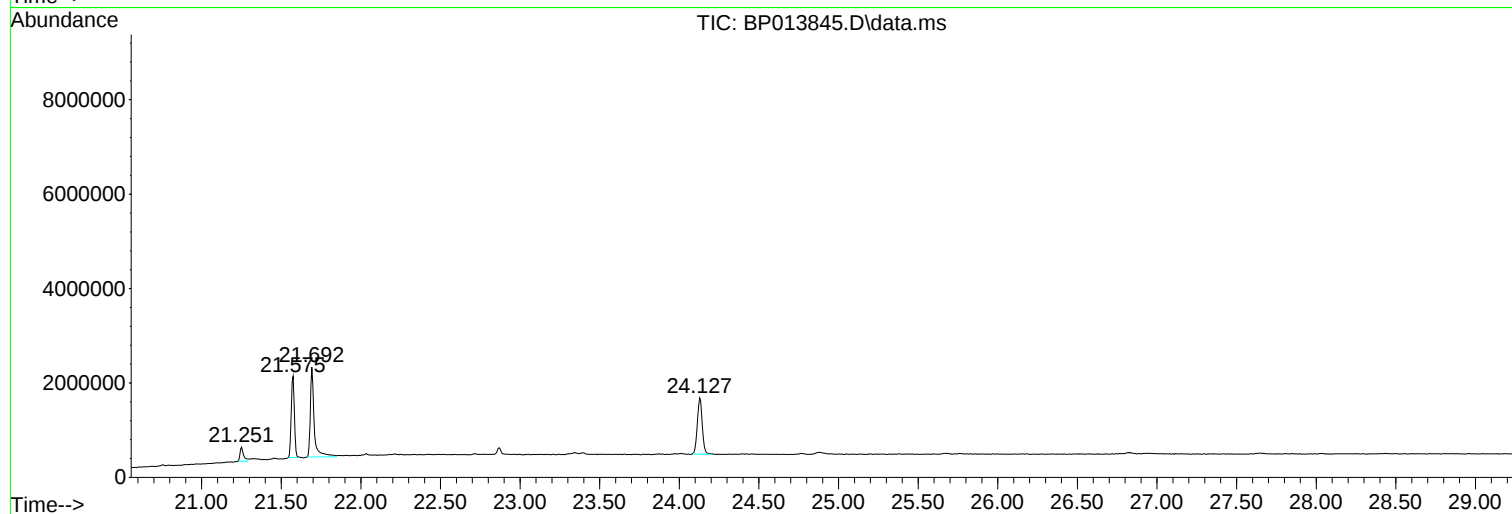
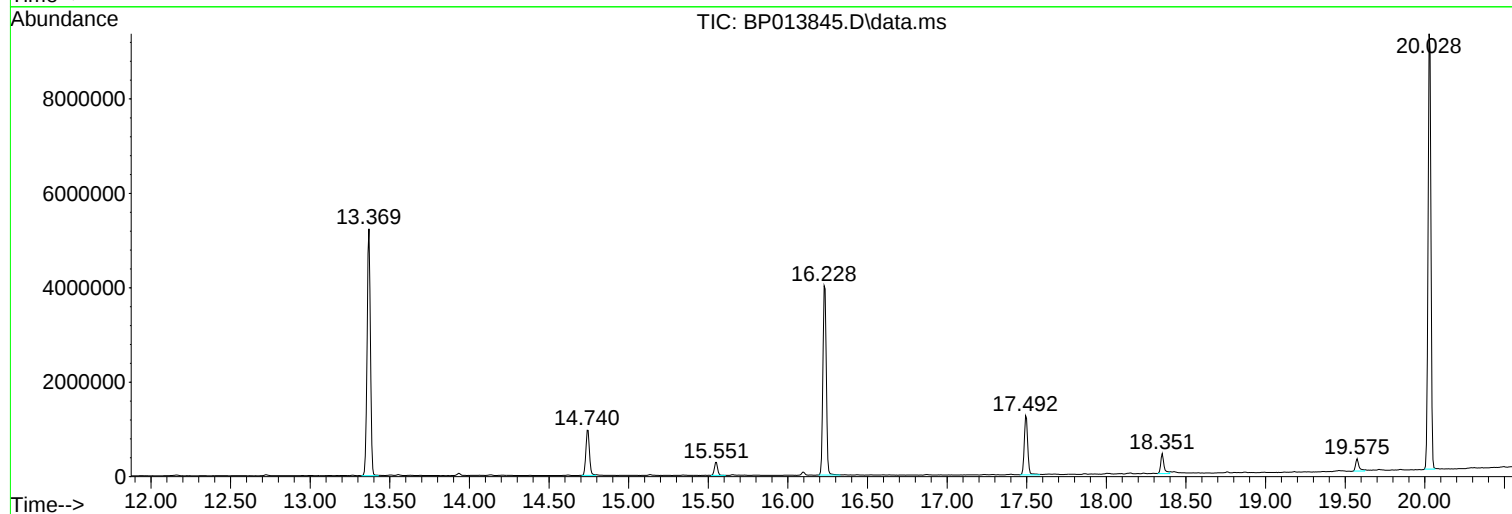
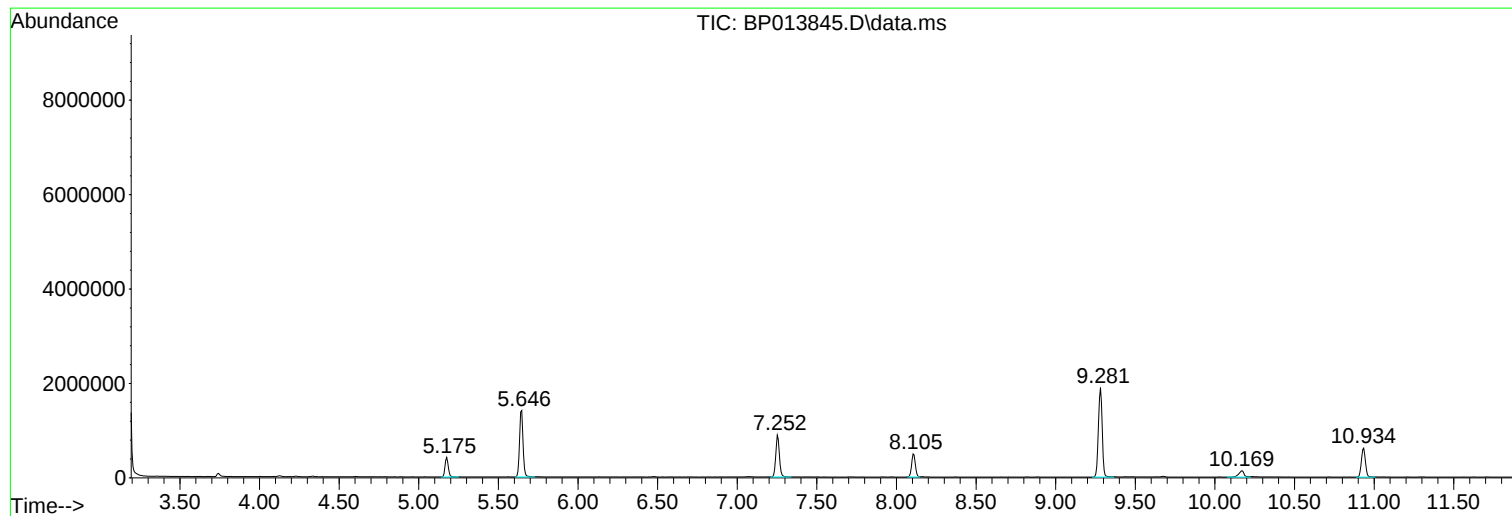
Sum of corrected areas: 48015033

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013845.D
Acq On : 17 Feb 2023 15:05
Operator : CG/JU
Sample : 01553-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TWP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.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_P\Data\BP021723\
Data File : BP013845.D
Acq On : 17 Feb 2023 15:05
Operator : CG/JU
Sample : 01553-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TWP-01

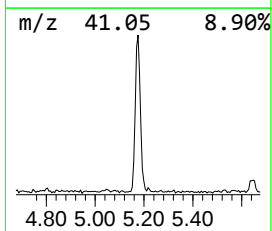
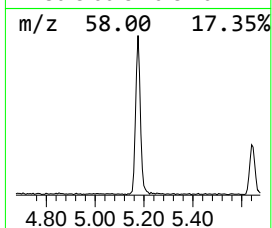
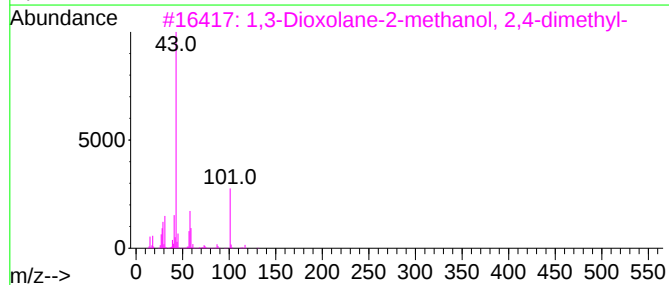
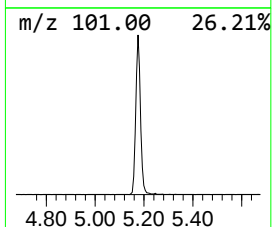
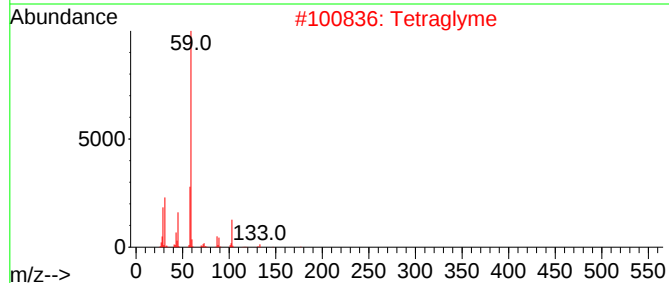
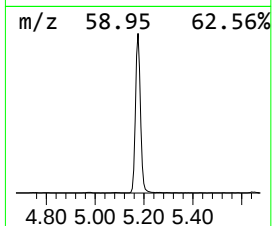
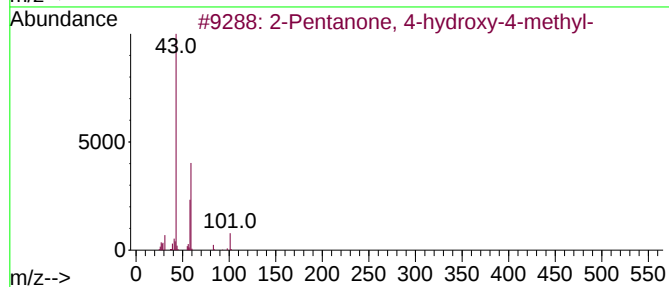
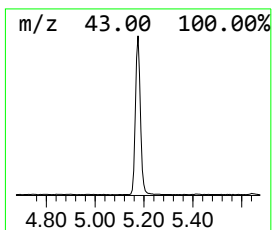
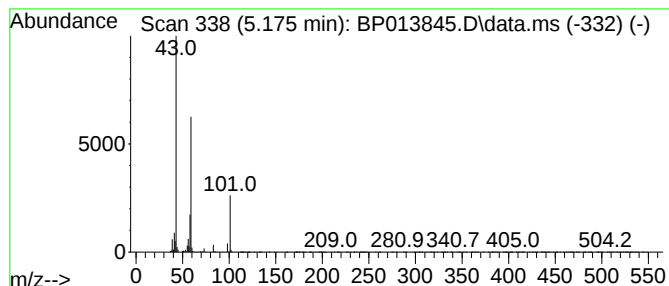
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.175	14.78 ng	580427	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Tetraglyme	222	C10H22O5	000143-24-8	25		
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013845.D
Acq On : 17 Feb 2023 15:05
Operator : CG/JU
Sample : 01553-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TWP-01

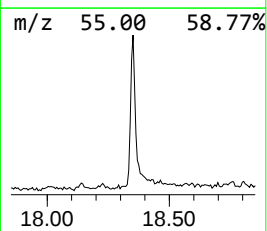
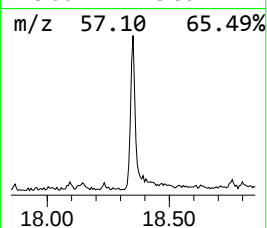
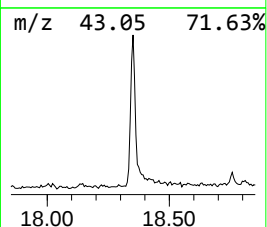
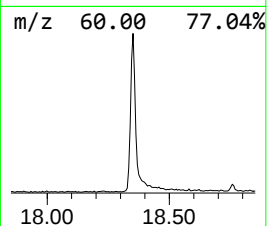
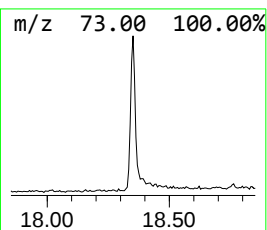
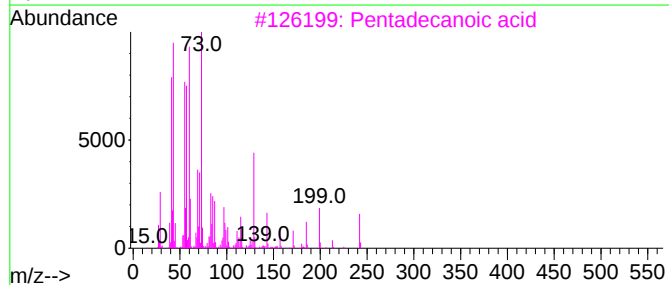
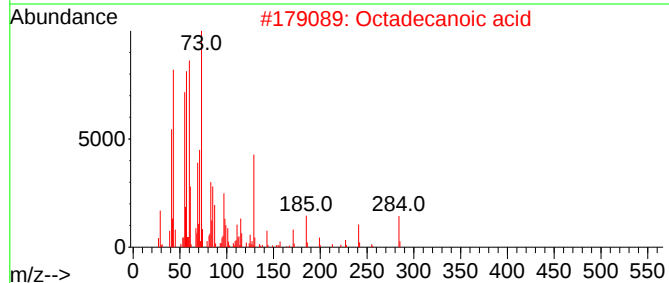
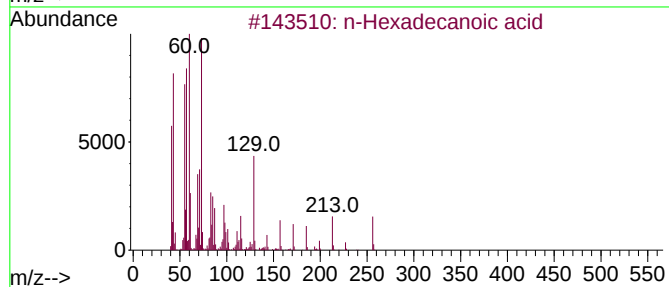
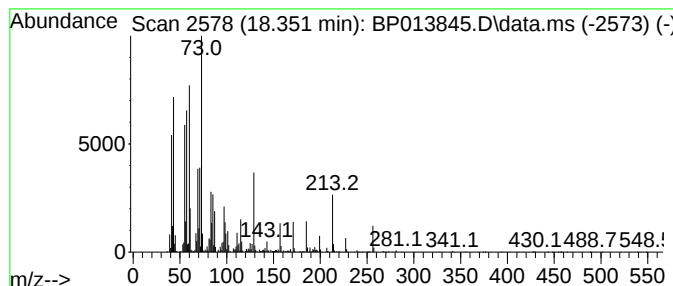
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.351	6.41 ng	607266	Phenanthrene-d10	17.493

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013845.D
Acq On : 17 Feb 2023 15:05
Operator : CG/JU
Sample : 01553-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TWP-01

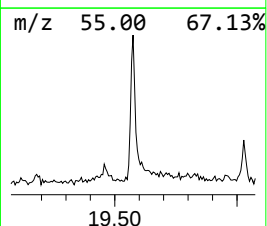
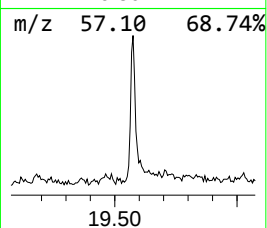
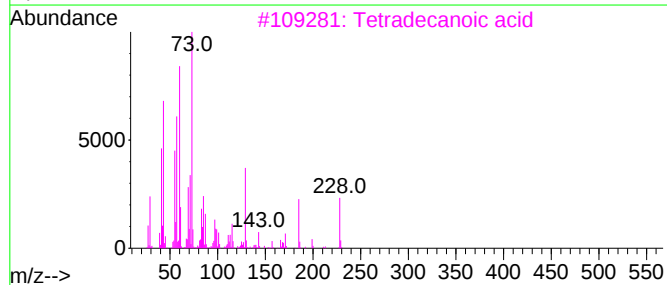
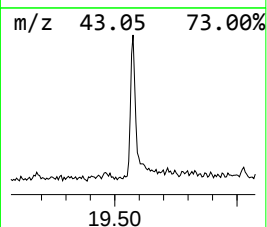
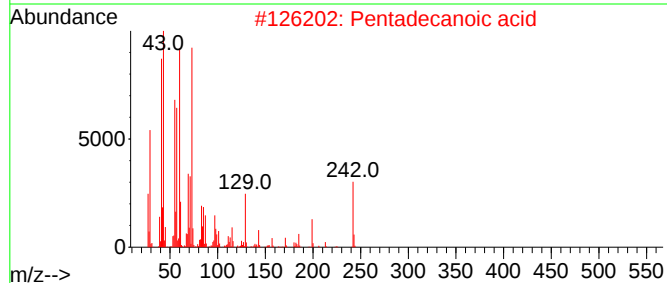
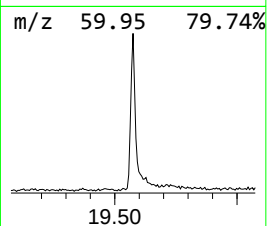
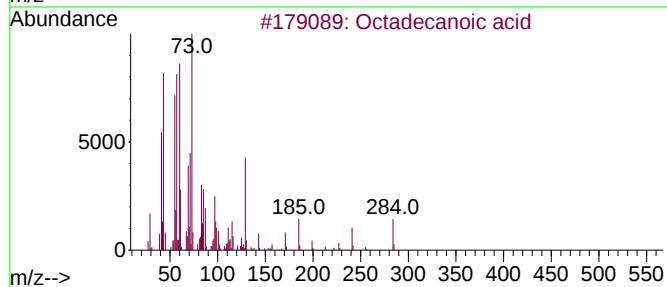
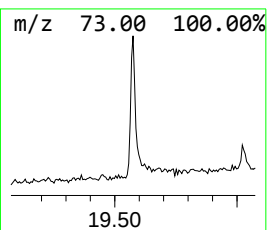
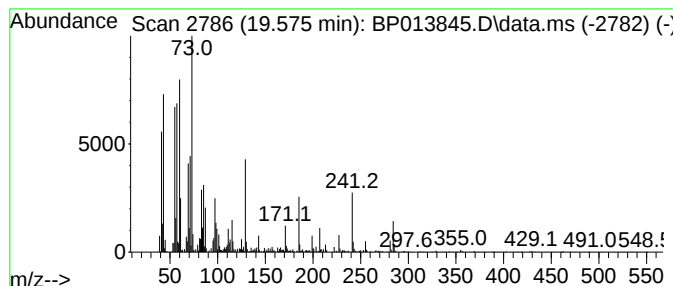
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.575	3.39 ng	392593	Chrysene-d12	21.575

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013845.D
Acq On : 17 Feb 2023 15:05
Operator : CG/JU
Sample : 01553-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TWP-01

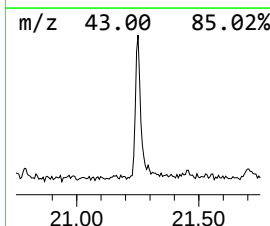
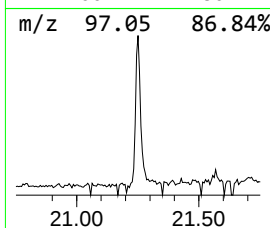
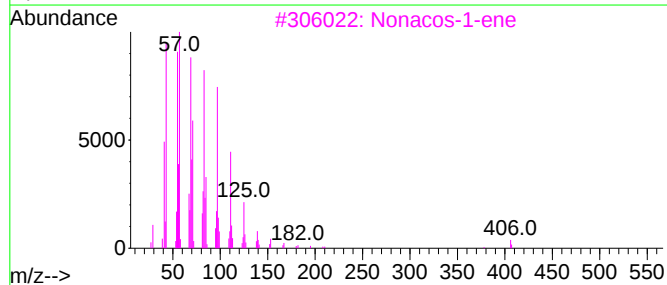
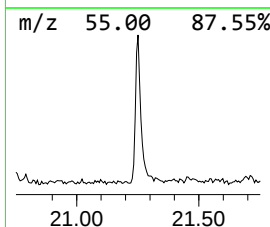
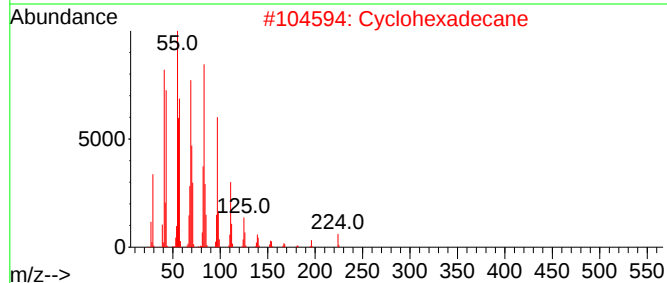
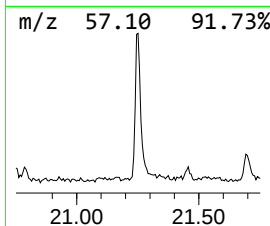
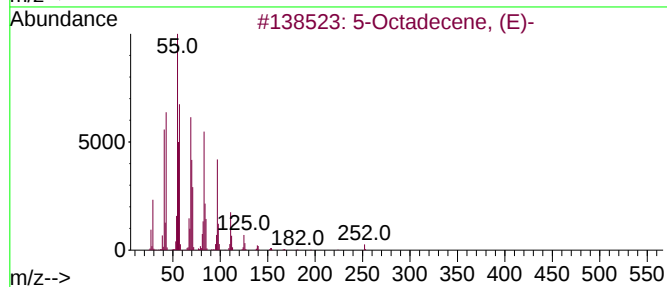
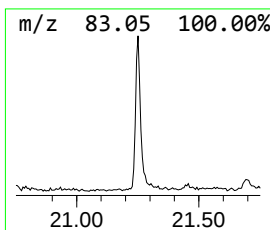
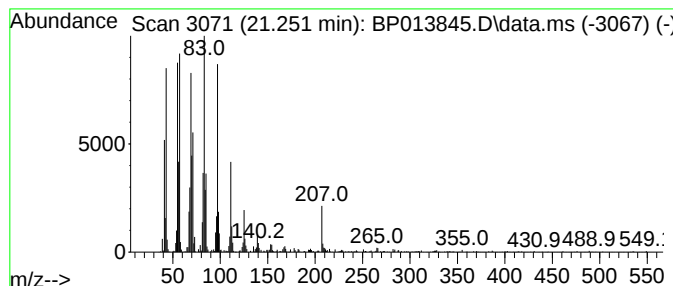
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 5-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.251	3.96 ng	458537	Chrysene-d12	21.575

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2			Cyclohexadecane	224	C16H32	000295-65-8	94
3			Nonacos-1-ene	406	C29H58	018835-35-3	94
4			Heptacos-1-ene	378	C27H54	015306-27-1	94
5			Pentacos-1-ene	350	C25H50	016980-85-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013845.D
Acq On : 17 Feb 2023 15:05
Operator : CG/JU
Sample : 01553-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TWP-01

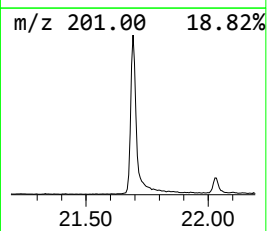
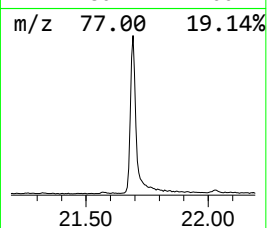
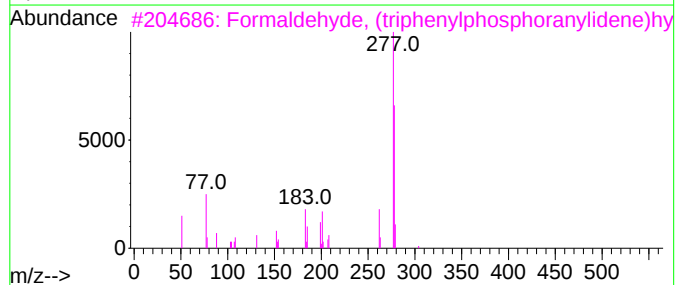
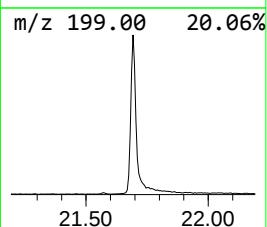
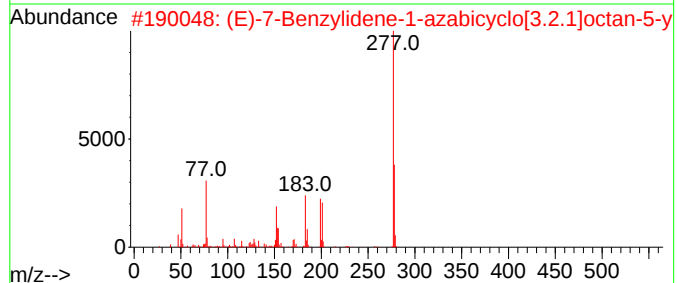
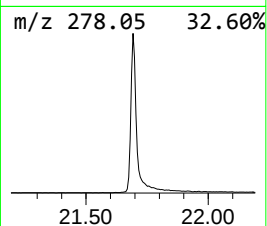
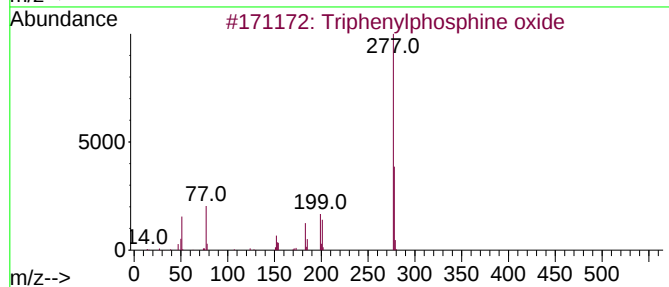
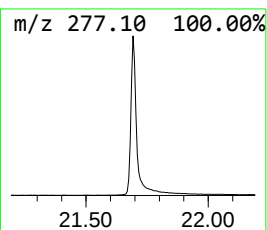
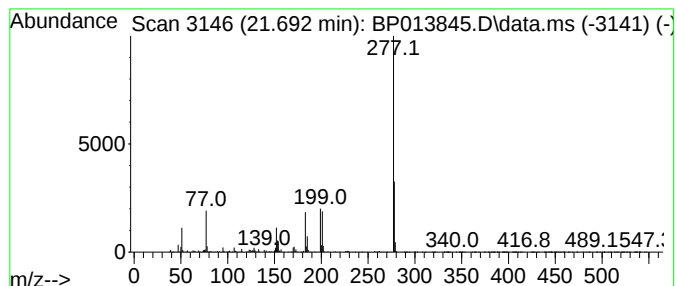
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.692	27.60 ng	3196700	Chrysene-d12	21.575

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	40
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	33
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013845.D
Acq On : 17 Feb 2023 15:05
Operator : CG/JU
Sample : 01553-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TWP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.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-...	5.175	14.8	ng	580427	1	8.105	785664	20.0
n-Hexadecanoic ...	18.351	6.4	ng	607266	4	17.493	1894880	20.0
Octadecanoic acid	19.575	3.4	ng	392593	5	21.575	2316100	20.0
5-Octadecene, (E)-	21.251	4.0	ng	458537	5	21.575	2316100	20.0
Triphenylphosph...	21.692	27.6	ng	3196700	5	21.575	2316100	20.0