

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
 Data File : BP005192.D
 Acq On : 06 Apr 2021 12:15
 Operator : CG/JU
 Sample : PB135526BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PB135526BL

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-BP032321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005192.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.299	369	376	386	rVB	463200	660139	46.79%	9.446%
2	6.881	638	645	656	rVB	406721	647144	45.87%	9.260%
3	7.693	777	783	793	rVB	74412	121275	8.60%	1.735%
4	8.857	973	981	992	rBV	245432	406192	28.79%	5.812%
5	10.487	1252	1258	1267	rVB	94089	157658	11.18%	2.256%
6	12.969	1671	1680	1688	rBV	614535	868851	61.59%	12.432%
7	14.351	1909	1915	1922	rBV2	139090	209259	14.83%	2.994%
8	15.851	2164	2170	2182	rBV	454070	654954	46.42%	9.372%
9	17.116	2376	2385	2392	rBV	178339	256288	18.17%	3.667%
10	18.016	2531	2538	2547	rBV	104564	173714	12.31%	2.486%
11	19.251	2744	2748	2759	rBV2	43614	68063	4.82%	0.974%
12	19.445	2777	2781	2788	rVB	13623	22673	1.61%	0.324%
13	19.510	2789	2792	2800	rVB4	8436	14994	1.06%	0.215%
14	19.692	2817	2823	2834	rBV	1117286	1410795	100.00%	20.187%
15	21.210	3076	3081	3088	rBV	229775	296378	21.01%	4.241%
16	21.363	3103	3107	3113	rVB4	22266	38968	2.76%	0.558%
17	23.492	3463	3469	3476	rVB2	150673	289291	20.51%	4.139%
18	23.851	3526	3530	3536	rVB4	41684	82702	5.86%	1.183%
19	24.957	3712	3718	3730	rVB3	74118	231755	16.43%	3.316%
20	26.280	3936	3943	3957	rVB3	107686	377516	26.76%	5.402%

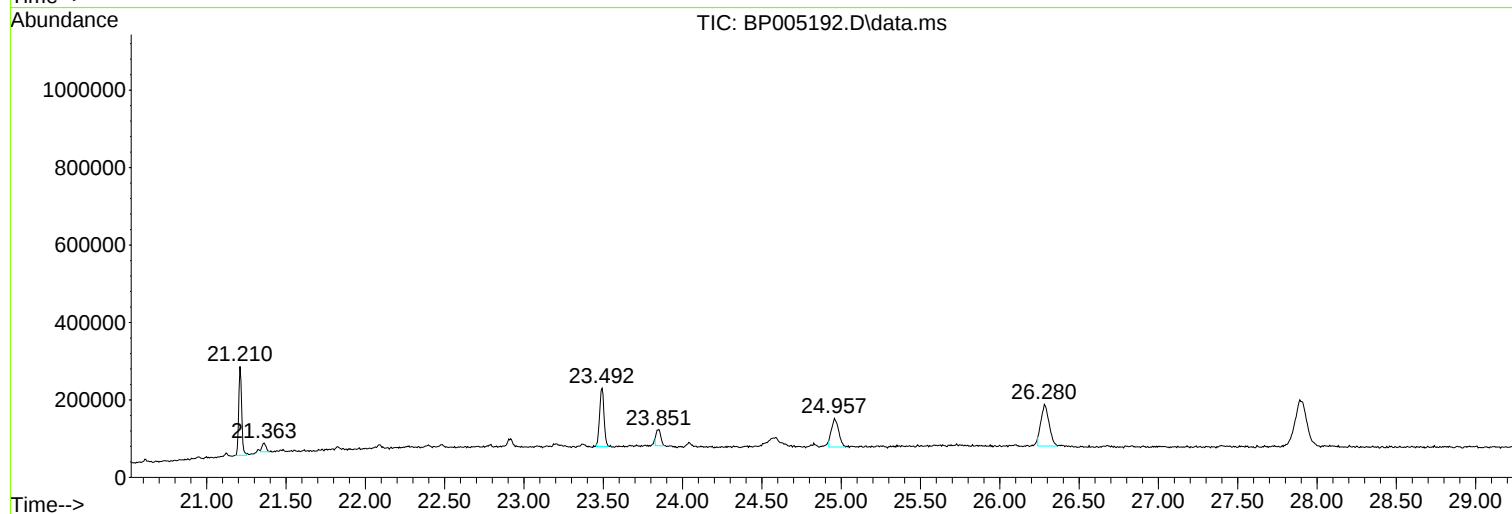
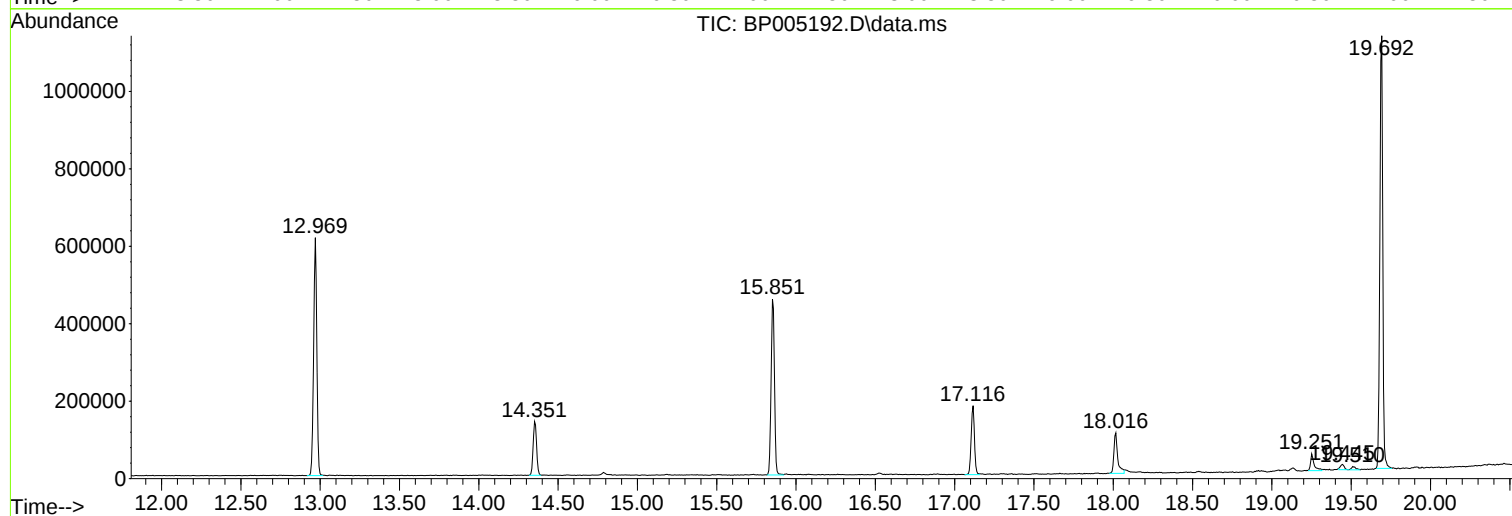
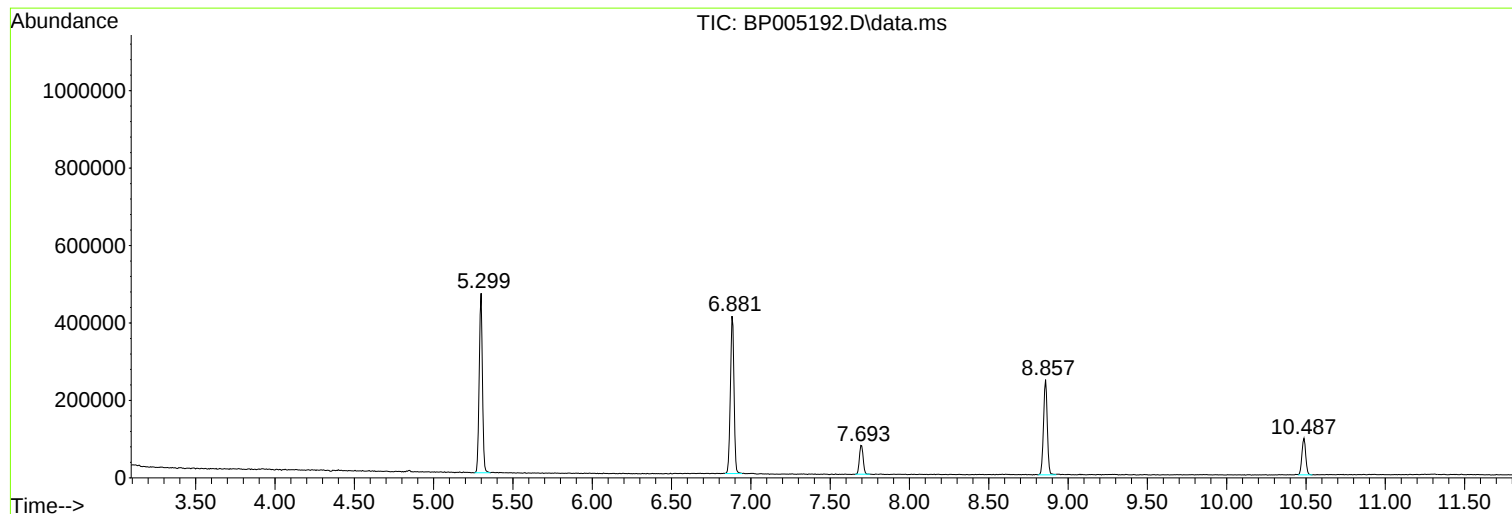
Sum of corrected areas: 6988609

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005192.D
Acq On : 06 Apr 2021 12:15
Operator : CG/JU
Sample : PB135526BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB135526BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005192.D
Acq On : 06 Apr 2021 12:15
Operator : CG/JU
Sample : PB135526BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB135526BL

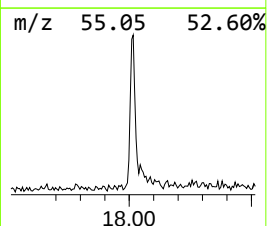
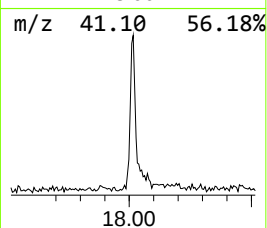
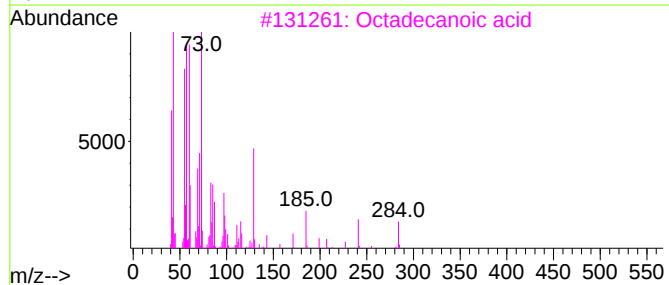
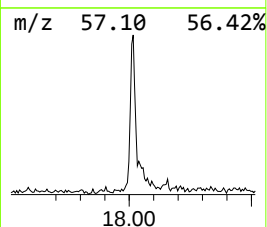
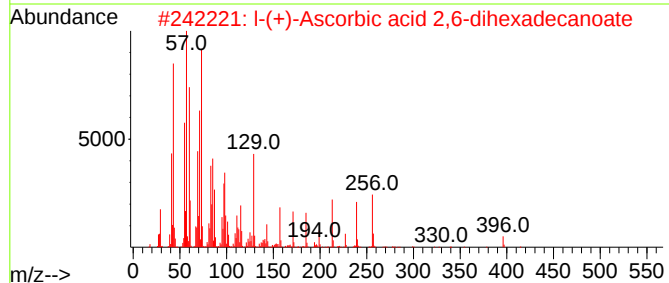
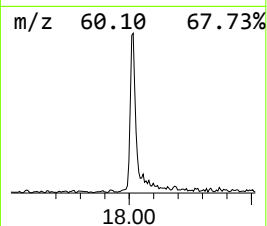
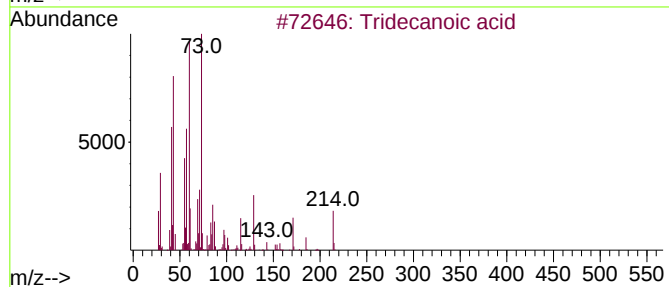
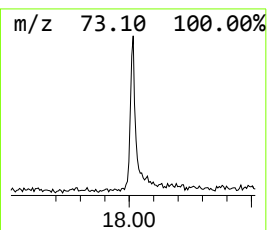
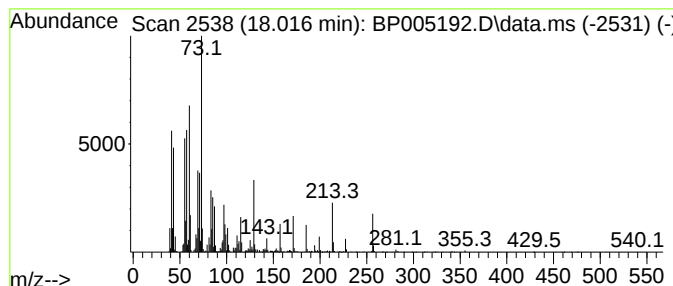
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.016	13.56 ng	173714	Phenanthrene-d10	17.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	83
2			l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	72
3			Octadecanoic acid	284	C18H36O2	000057-11-4	70
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005192.D
Acq On : 06 Apr 2021 12:15
Operator : CG/JU
Sample : PB135526BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB135526BL

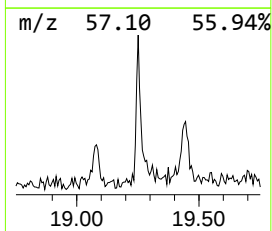
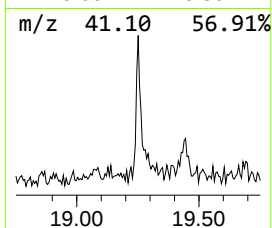
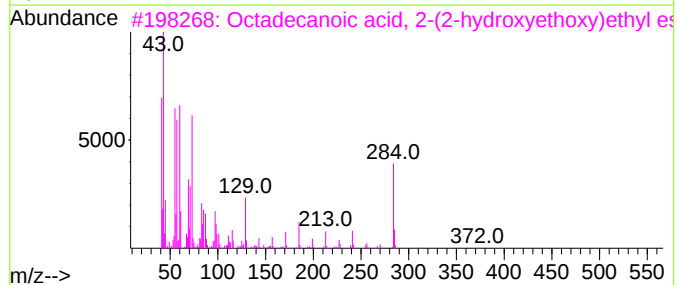
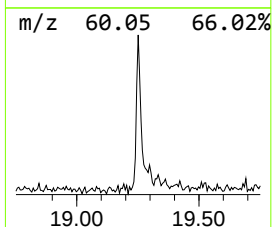
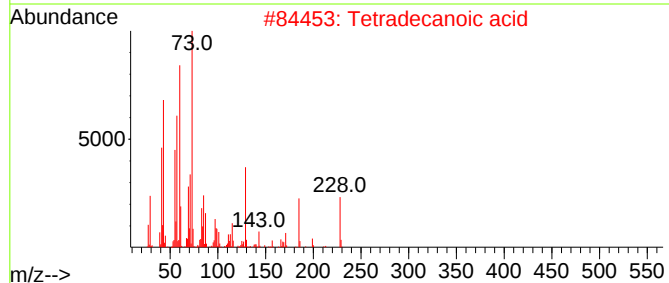
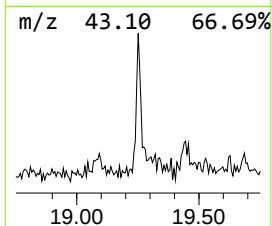
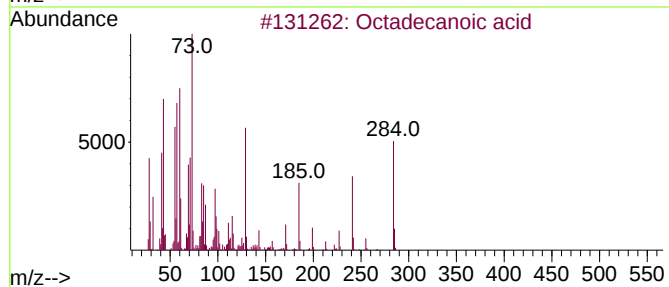
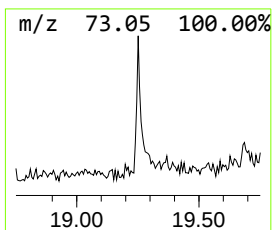
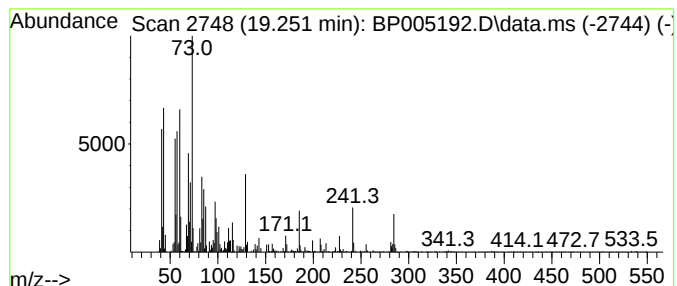
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.251	4.59 ng	68063	Chrysene-d12	21.210

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5		n-Decanoic acid	172	C10H20O2	000334-48-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005192.D
Acq On : 06 Apr 2021 12:15
Operator : CG/JU
Sample : PB135526BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

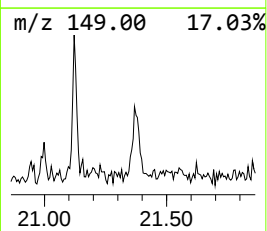
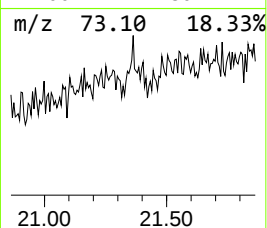
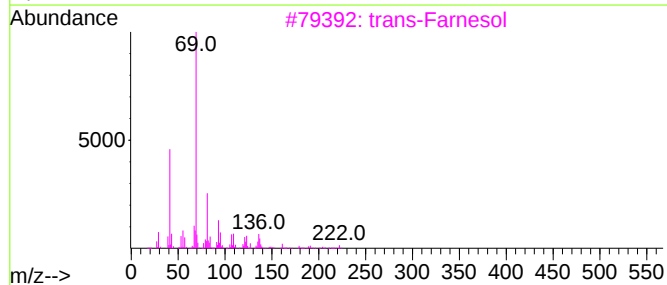
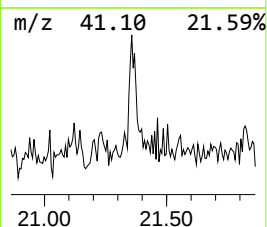
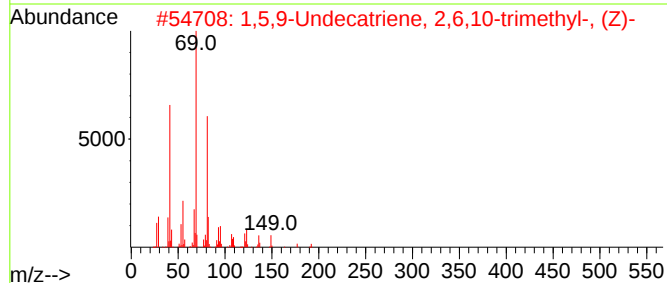
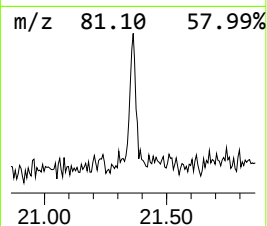
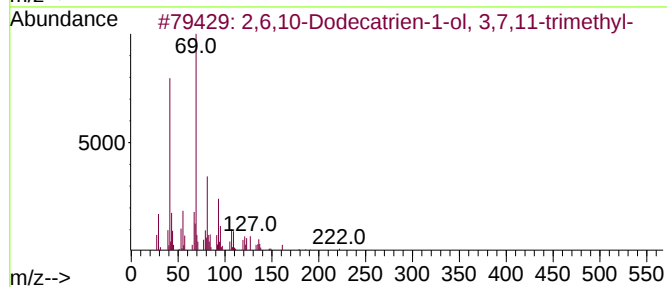
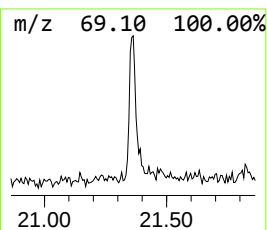
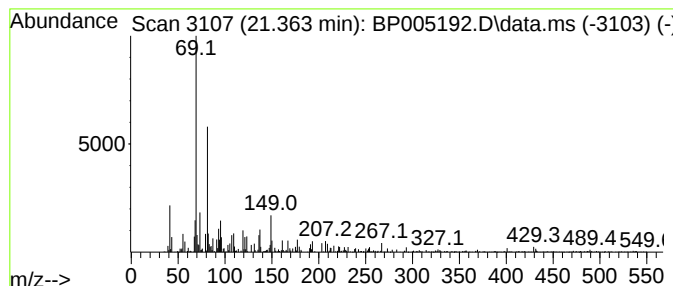
Instrument :
BNA_P
ClientSampleId :
PB135526BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.363	2.63 ng	38968	Chrysene-d12	21.210	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	68
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	68
3	trans-Farnesol	222	C15H26O	000106-28-5	68
4	Supraene	410	C30H50	007683-64-9	64
5	Propane, 1-chloro-3-diethylboryl...	190	C9H20BClO	1000150-50-3	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005192.D
Acq On : 06 Apr 2021 12:15
Operator : CG/JU
Sample : PB135526BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB135526BL

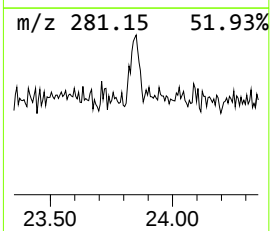
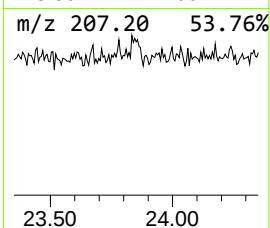
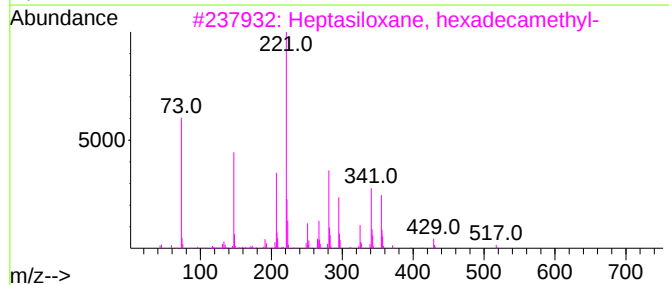
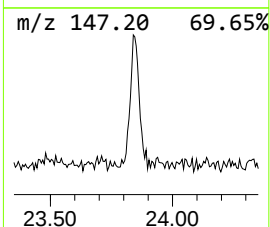
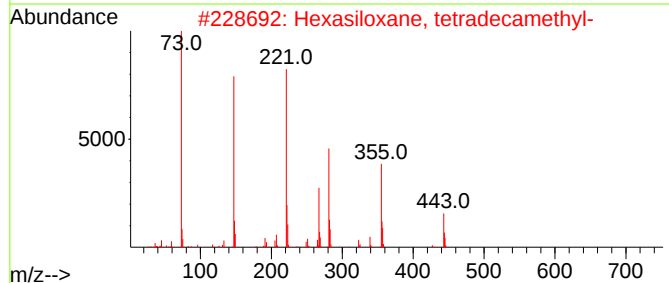
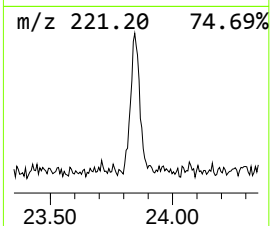
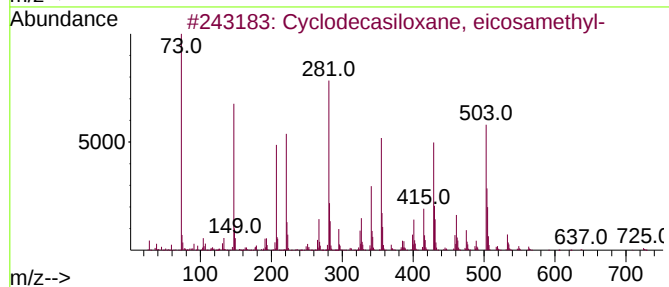
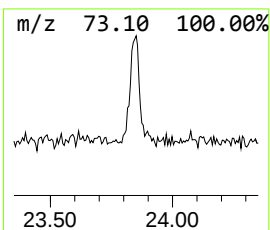
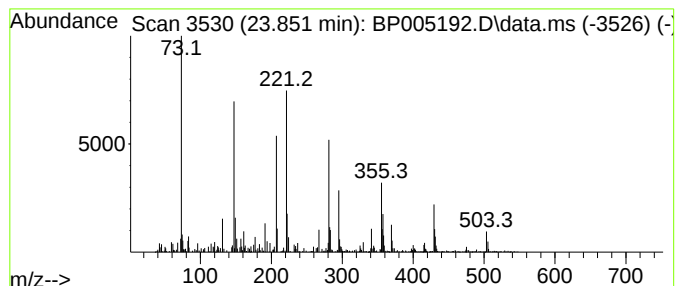
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclodecasiloxane, eicosame... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.851	5.72 ng	82702	Perylene-d12	23.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	76
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	47
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
4			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	32
5			Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005192.D
Acq On : 06 Apr 2021 12:15
Operator : CG/JU
Sample : PB135526BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB135526BL

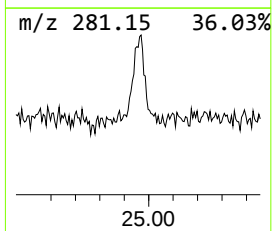
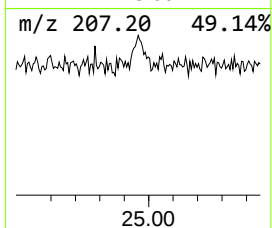
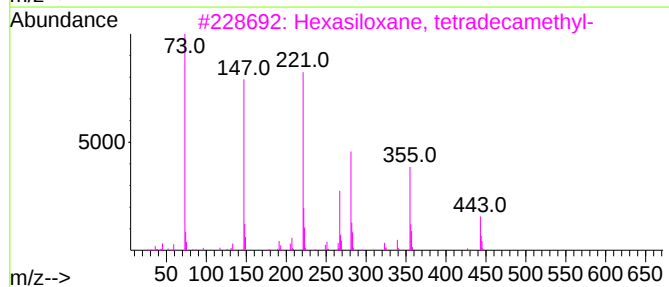
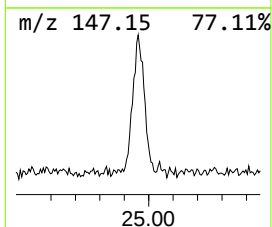
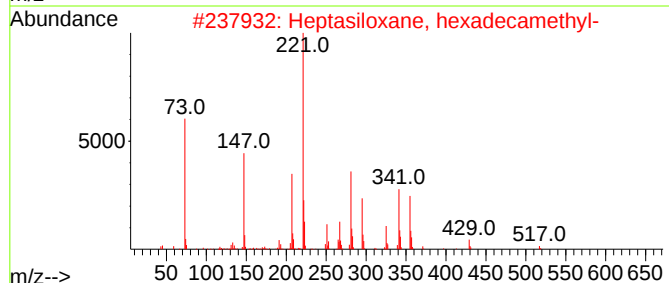
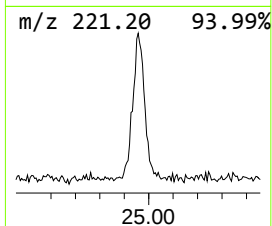
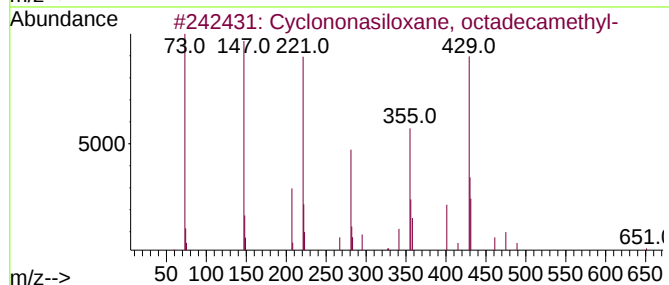
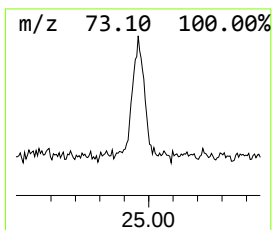
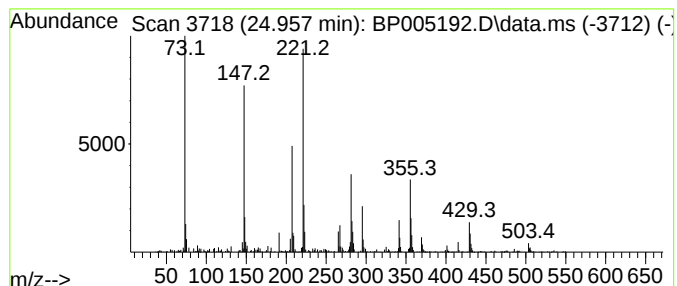
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclononasiloxane, octadeca... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.957	16.02 ng	231755	Perylene-d12	23.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	83
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	74
3			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	53
4			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	22
5			Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005192.D
Acq On : 06 Apr 2021 12:15
Operator : CG/JU
Sample : PB135526BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB135526BL

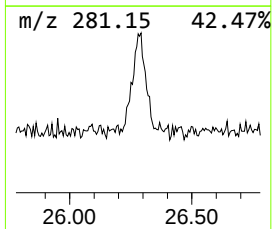
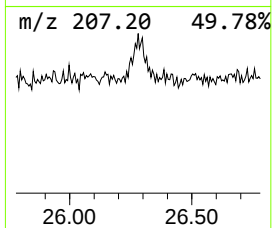
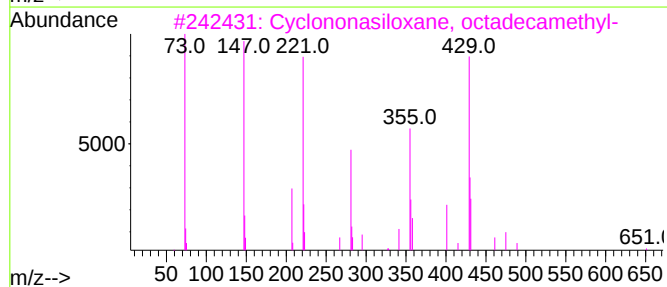
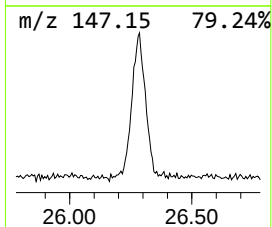
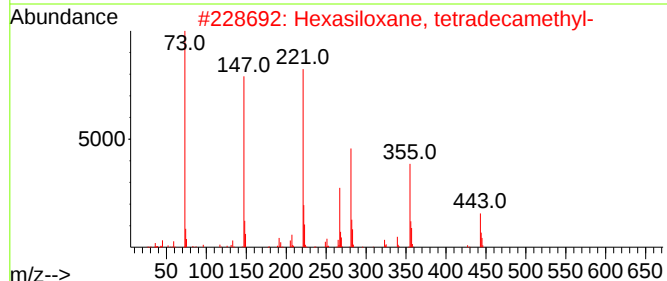
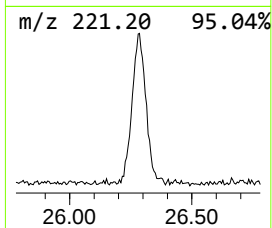
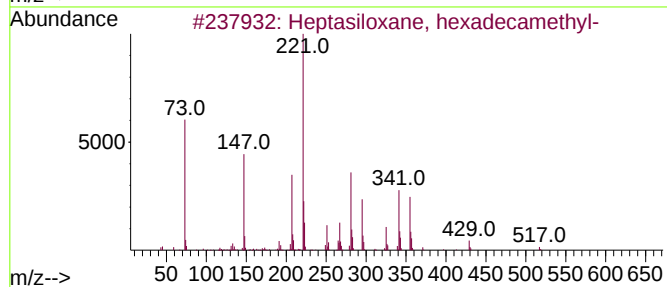
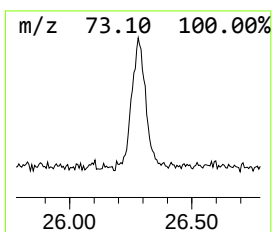
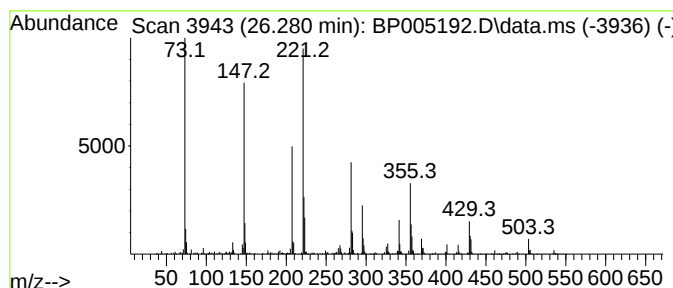
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptasiloxane, hexadecamethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.280	26.10 ng	377516	Perylene-d12	23.492

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	64
2		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	58
3		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	37
4		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25
5		Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005192.D
Acq On : 06 Apr 2021 12:15
Operator : CG/JU
Sample : PB135526BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB135526BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Tridecanoic acid	18.016	13.6	ng	173714	4	17.116	256288	20.0
Octadecanoic acid	19.251	4.6	ng	68063	5	21.210	296378	20.0
2,6,10-Dodecatr...	21.363	2.6	ng	38968	5	21.210	296378	20.0
Cyclodecasiloxa...	23.851	5.7	ng	82702	6	23.492	289291	20.0
Cyclononasiloxa...	24.957	16.0	ng	231755	6	23.492	289291	20.0
Heptasiloxane, ...	26.280	26.1	ng	377516	6	23.492	289291	20.0