

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
 Data File : BP007056.D
 Acq On : 20 Sep 2021 18:35
 Operator : CG/JU
 Sample : M3687-36
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A002145

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-BP091621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007056.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.481	400	407	420	rBV	3691676	5368061	39.64%	7.920%
2	7.069	670	677	691	rBV	3422678	5507328	40.67%	8.125%
3	7.905	812	819	826	rBV	1050905	1658423	12.25%	2.447%
4	9.069	1008	1017	1027	rBV	2011687	3466274	25.59%	5.114%
5	10.487	1251	1258	1273	rBV	630538	1102771	8.14%	1.627%
6	10.704	1288	1295	1303	rBV	1336934	2244100	16.57%	3.311%
7	13.163	1704	1713	1725	rBV	5803410	8561337	63.22%	12.631%
8	14.534	1939	1946	1957	rVB	2006050	2968576	21.92%	4.380%
9	16.022	2192	2199	2218	rVB	4436816	6490747	47.93%	9.576%
10	17.281	2406	2413	2425	rBV	2584484	3633126	26.83%	5.360%
11	18.169	2558	2564	2592	rBV	916575	1724958	12.74%	2.545%
12	19.398	2768	2773	2789	rBV2	520278	925242	6.83%	1.365%
13	19.833	2842	2847	2854	rBV	10715664	13543152	100.00%	19.981%
14	21.074	3054	3058	3066	rBV	466072	668029	4.93%	0.986%
15	21.363	3102	3107	3116	rBV	3186069	4240147	31.31%	6.256%
16	22.621	3316	3321	3327	rVB	762817	1082447	7.99%	1.597%
17	23.774	3510	3517	3536	rVB2	2138654	4597125	33.94%	6.782%

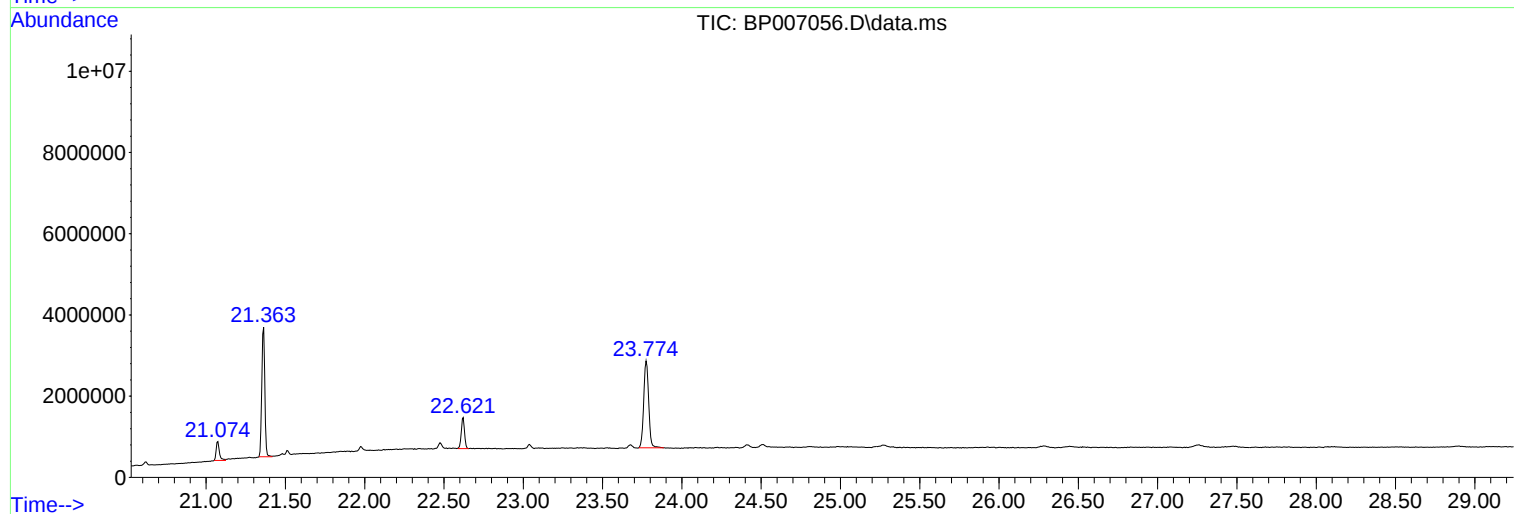
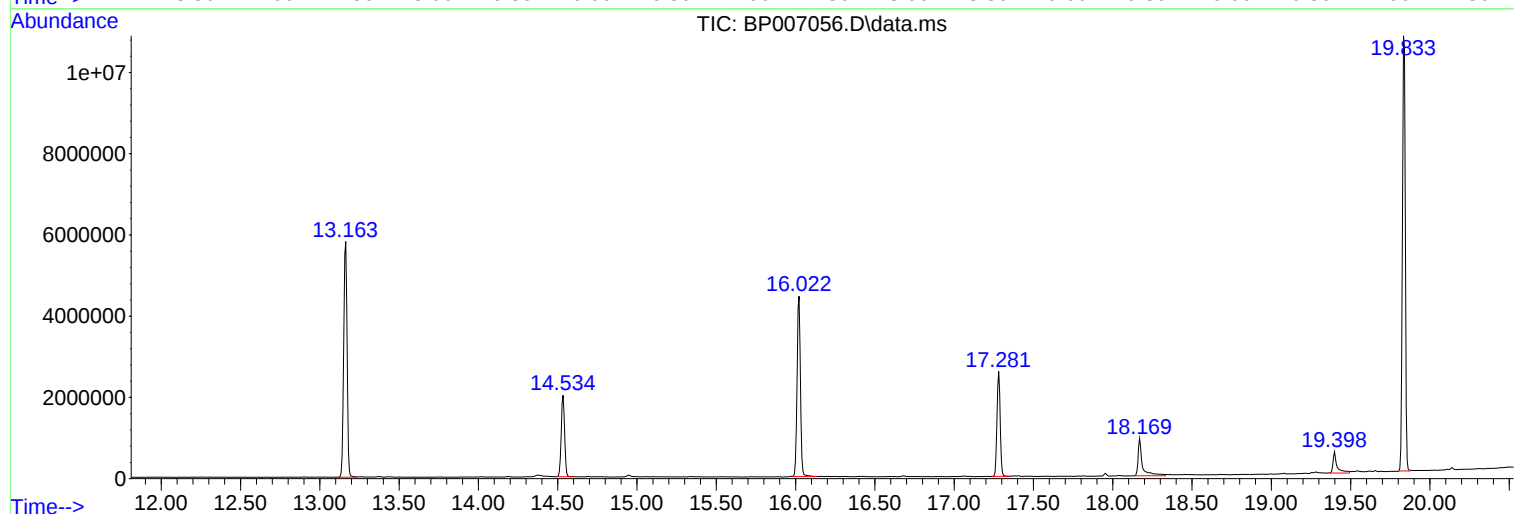
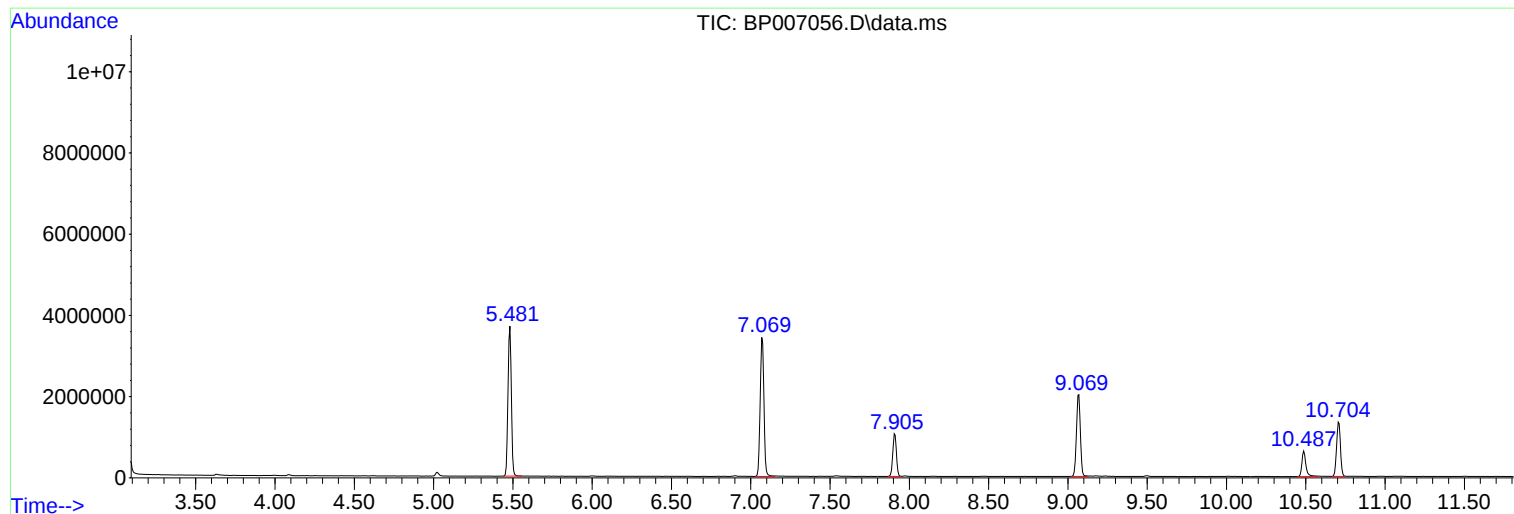
Sum of corrected areas: 67781843

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007056.D
Acq On : 20 Sep 2021 18:35
Operator : CG/JU
Sample : M3687-36
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A002145

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.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\BP092021\
Data File : BP007056.D
Acq On : 20 Sep 2021 18:35
Operator : CG/JU
Sample : M3687-36
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A002145

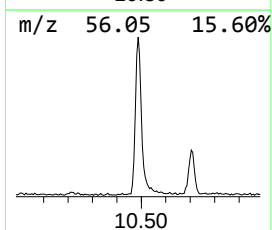
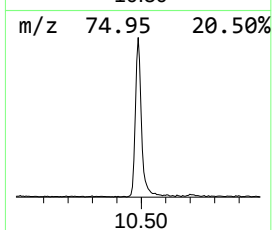
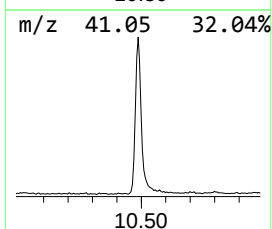
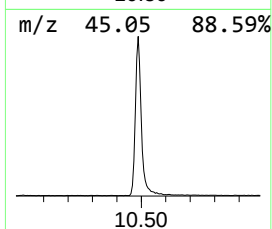
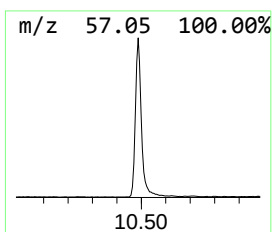
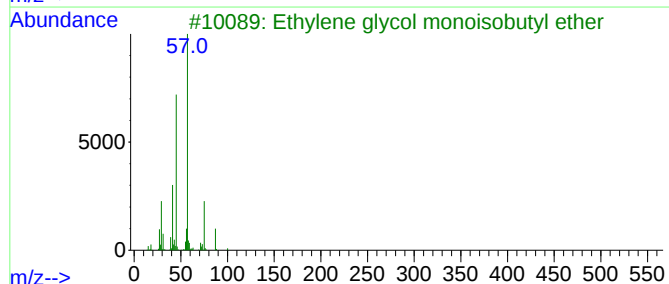
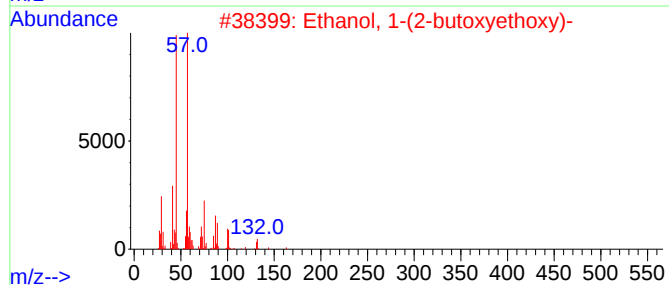
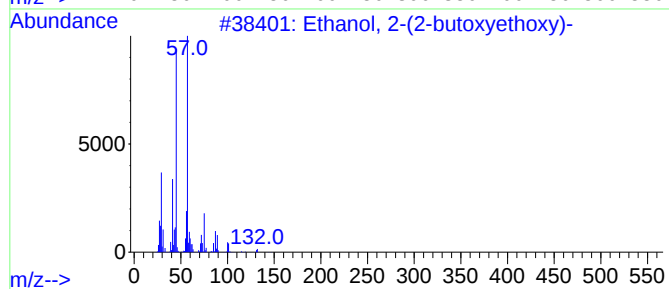
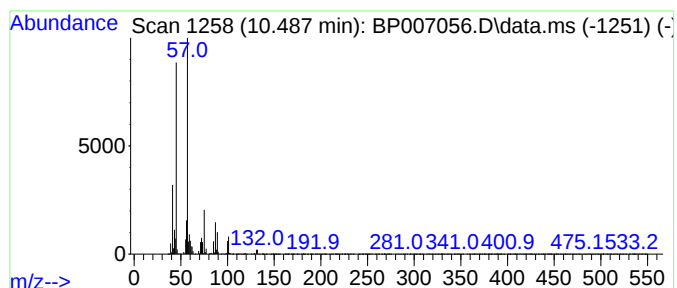
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.487	9.83 ng	1102770	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007056.D
Acq On : 20 Sep 2021 18:35
Operator : CG/JU
Sample : M3687-36
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A002145

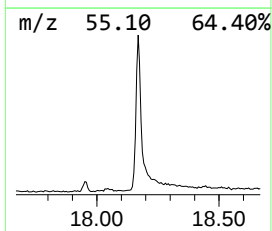
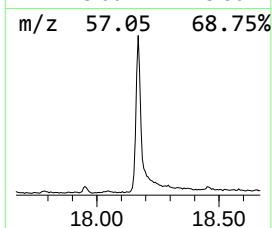
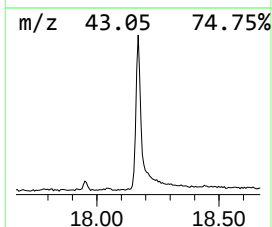
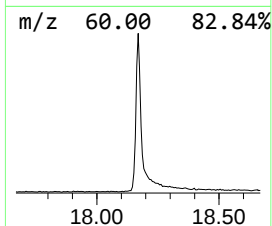
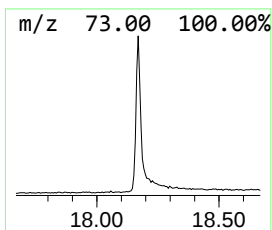
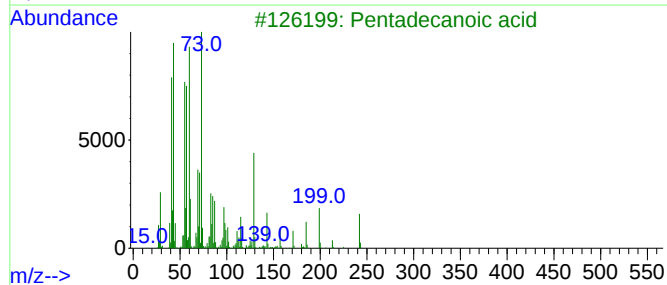
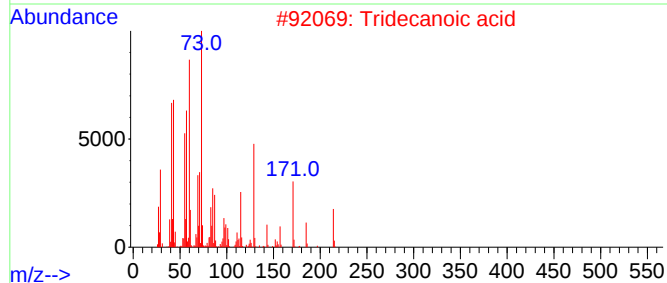
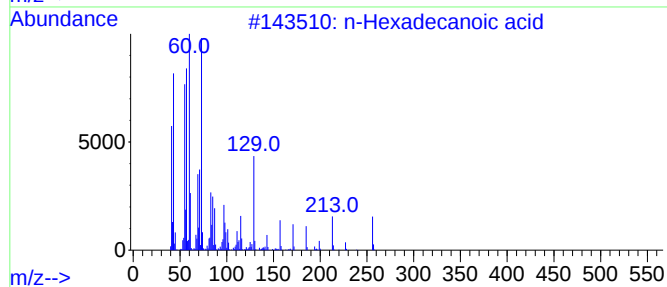
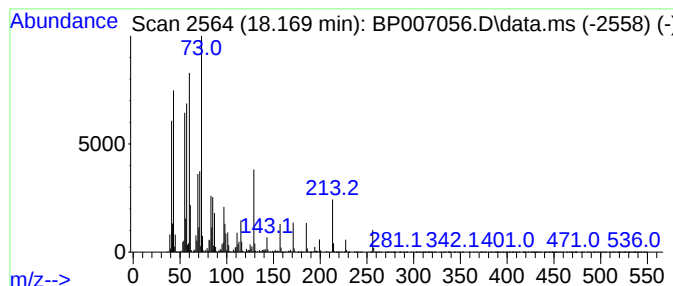
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	9.50 ng	1724960	Phenanthrene-d10	17.281

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	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007056.D
Acq On : 20 Sep 2021 18:35
Operator : CG/JU
Sample : M3687-36
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A002145

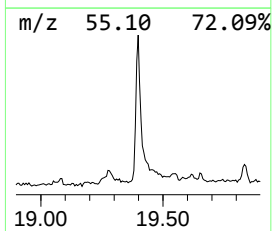
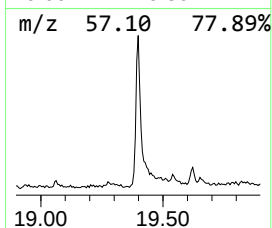
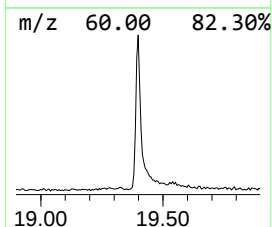
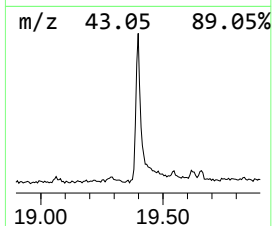
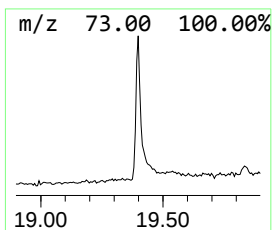
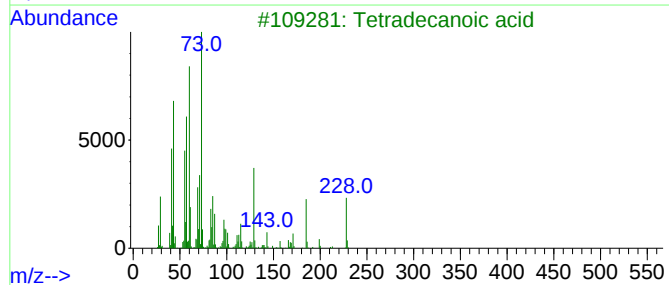
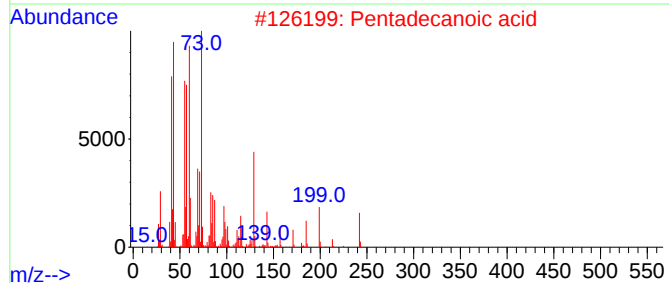
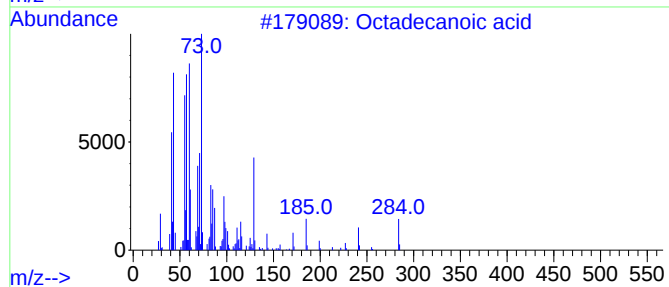
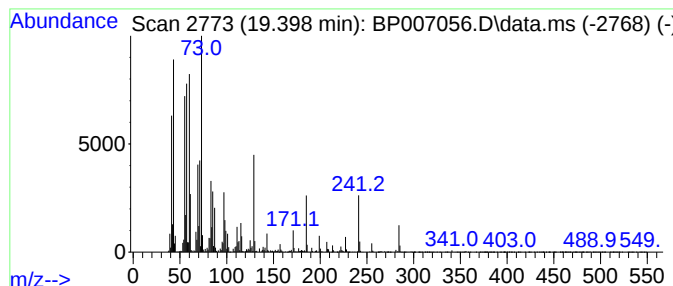
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	4.36 ng	925242	Chrysene-d12	21.363

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	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007056.D
Acq On : 20 Sep 2021 18:35
Operator : CG/JU
Sample : M3687-36
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A002145

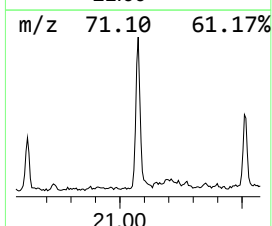
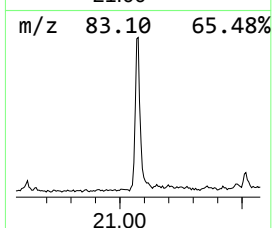
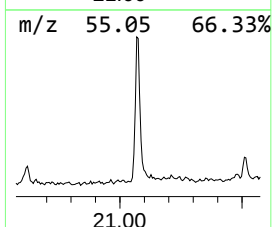
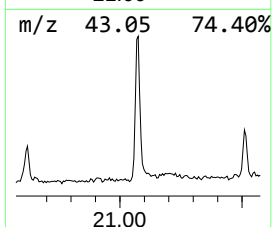
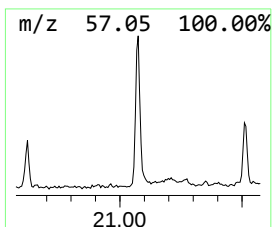
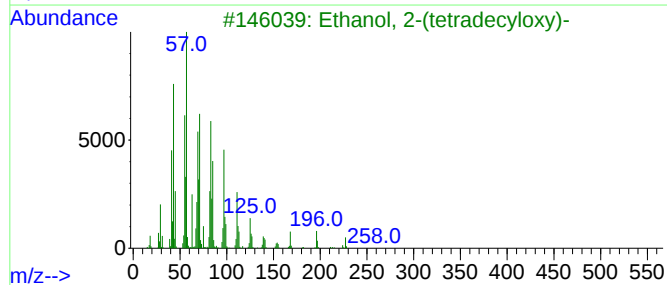
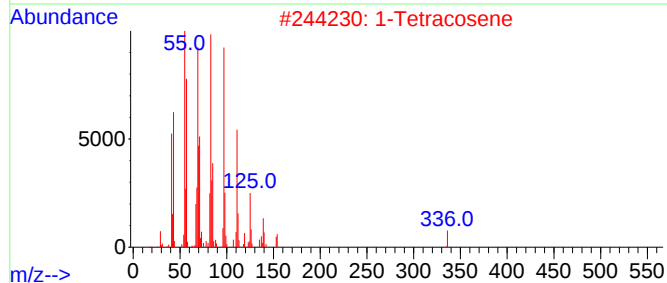
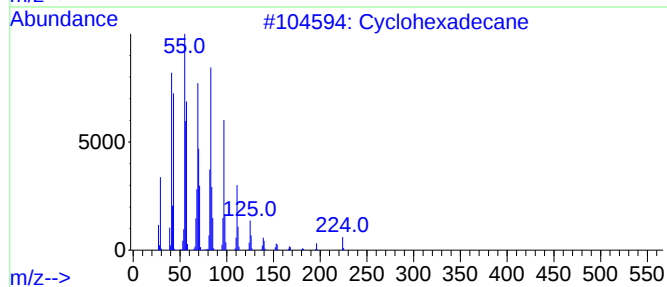
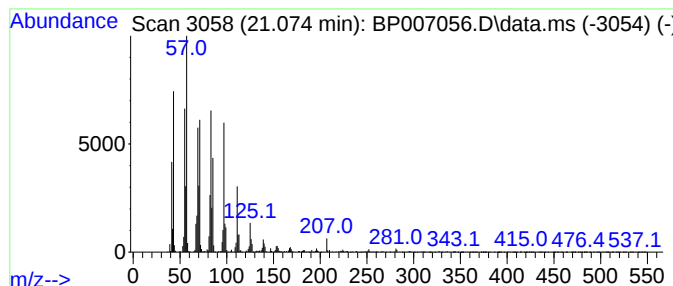
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	3.15 ng	668029	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	99
2			1-Tetracosene	336	C24H48	010192-32-2	97
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	95
4			5-Octadecene, (E)-	252	C18H36	007206-21-5	95
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007056.D
Acq On : 20 Sep 2021 18:35
Operator : CG/JU
Sample : M3687-36
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A002145

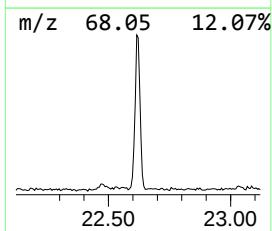
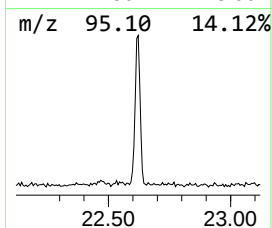
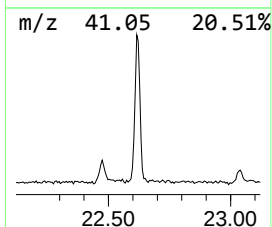
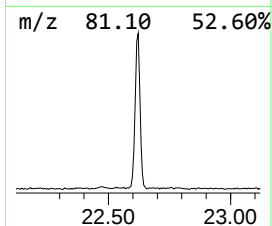
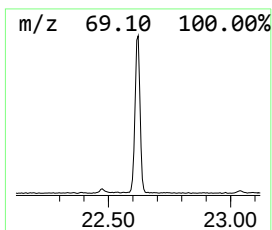
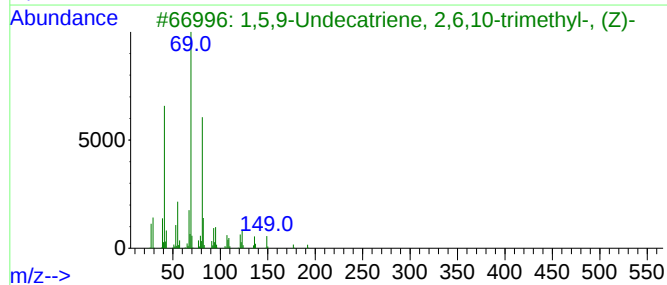
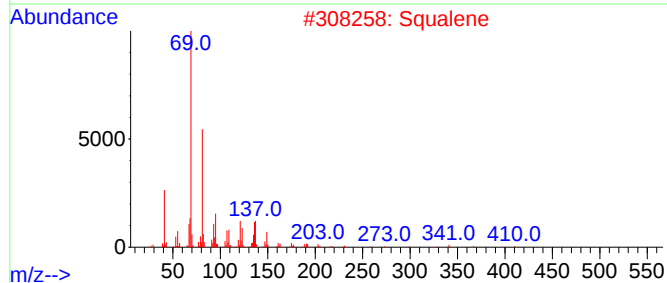
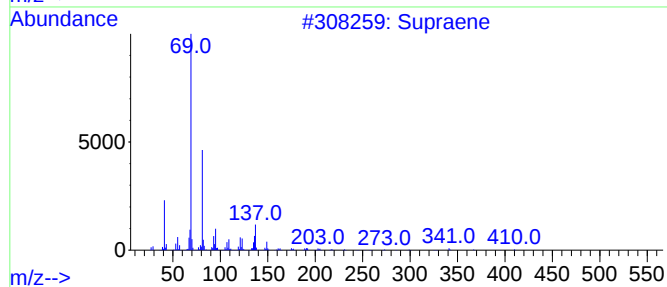
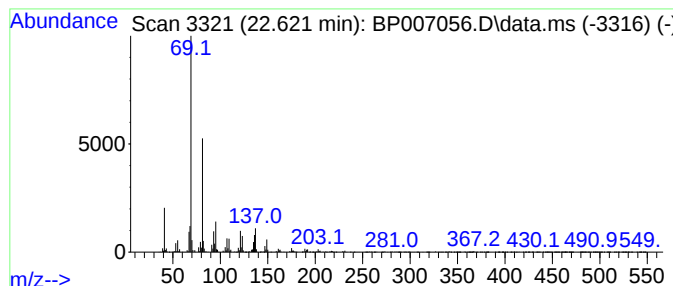
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.621	4.71 ng	1082450	Perylene-d12	23.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	86
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	86
4			Umbelliprenin	366	C24H30O3	023838-17-7	72
5			trans-Farnesol	222	C15H26O	000106-28-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
Data File : BP007056.D
Acq On : 20 Sep 2021 18:35
Operator : CG/JU
Sample : M3687-36
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A002145

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.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
Ethanol, 2-(2-b...	10.487	9.8	ng	1102770	2	10.704	2244100	20.0
n-Hexadecanoic ...	18.169	9.5	ng	1724960	4	17.281	3633130	20.0
Octadecanoic acid	19.398	4.4	ng	925242	5	21.363	4240150	20.0
Cyclohexadecane	21.074	3.1	ng	668029	5	21.363	4240150	20.0
Supraene	22.621	4.7	ng	1082450	6	23.774	4597130	20.0