

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
 Data File : BP011815.D
 Acq On : 27 Sep 2022 14:50
 Operator : CG/JU
 Sample : N4835-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 529317-4

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-BP092122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011815.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.052	6	11	36	rVB	9178764	14161541	54.16%	10.491%
2	5.469	416	422	437	rBV	2882728	4394495	16.81%	3.256%
3	7.069	686	694	709	rBV	1571950	2639565	10.10%	1.955%
4	7.911	829	837	844	rBV	1476801	2390463	9.14%	1.771%
5	9.081	1028	1036	1052	rBV	4489671	7662035	29.30%	5.676%
6	10.499	1270	1277	1299	rBV	716458	1415253	5.41%	1.048%
7	10.722	1306	1315	1334	rBV	2038220	3526114	13.49%	2.612%
8	13.181	1725	1733	1748	rBV	11564163	17783848	68.02%	13.175%
9	14.551	1957	1966	1982	rBV	3206991	4942742	18.90%	3.662%
10	16.045	2214	2220	2241	rBV	8604042	12494391	47.79%	9.256%
11	17.310	2428	2435	2446	rBV	4324940	6041945	23.11%	4.476%
12	17.975	2544	2548	2554	rBV	254852	321318	1.23%	0.238%
13	18.192	2580	2585	2605	rBV	893220	1999981	7.65%	1.482%
14	19.428	2790	2795	2816	rBV	2677526	4991153	19.09%	3.698%
15	19.869	2864	2870	2875	rBV	20306633	26146328	100.00%	19.370%
16	21.104	3076	3080	3088	rBV	467822	818188	3.13%	0.606%
17	21.392	3124	3129	3139	rBV	5081201	6490133	24.82%	4.808%
18	21.516	3145	3150	3171	rBV	6757777	10146176	38.81%	7.516%
19	23.839	3538	3545	3555	rVB2	2941780	6246789	23.89%	4.628%
20	24.727	3694	3696	3698	rBV	271607	373289	1.43%	0.277%

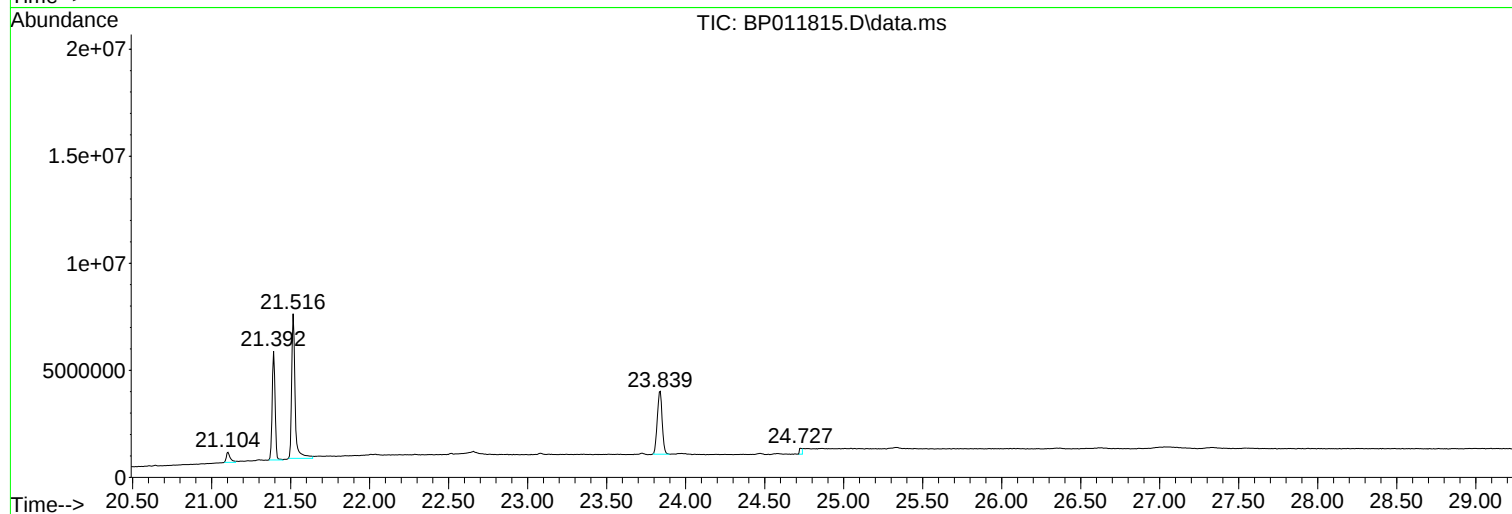
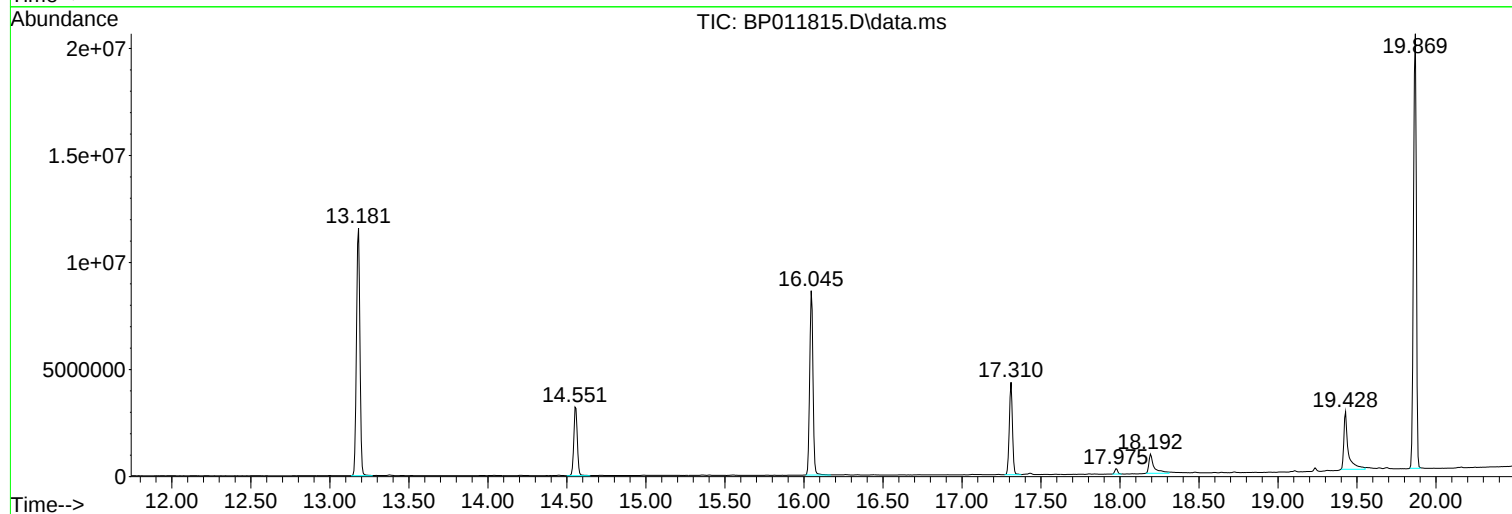
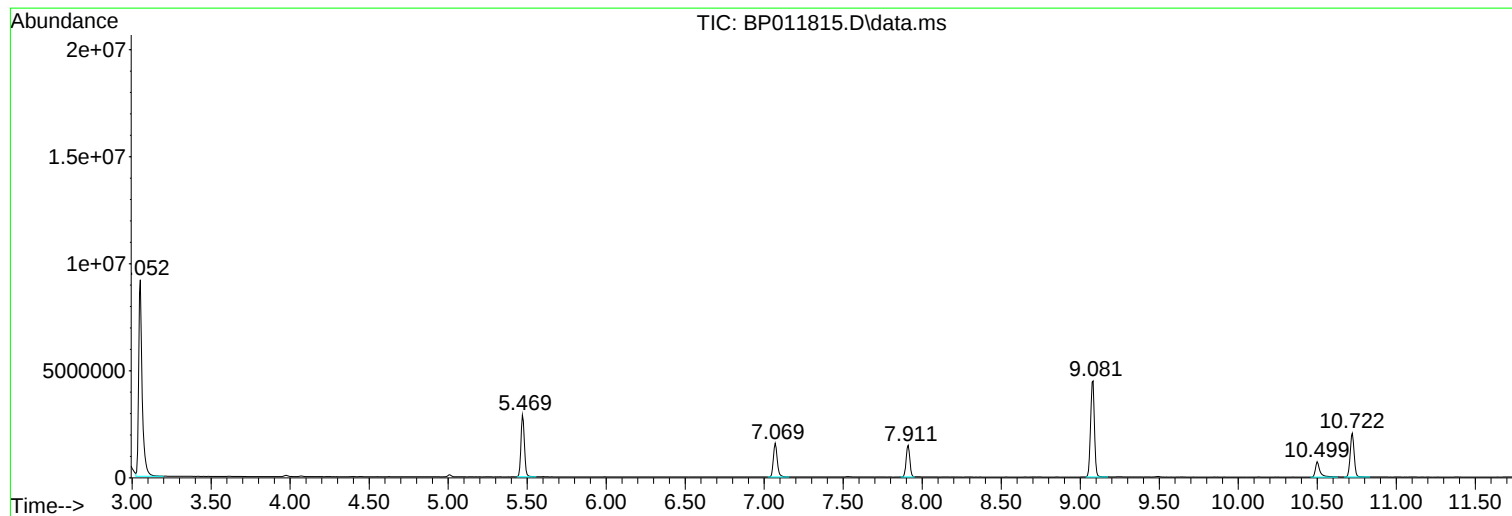
Sum of corrected areas: 134985747

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011815.D
Acq On : 27 Sep 2022 14:50
Operator : CG/JU
Sample : N4835-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
529317-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.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\BP092722\
Data File : BP011815.D
Acq On : 27 Sep 2022 14:50
Operator : CG/JU
Sample : N4835-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
529317-4

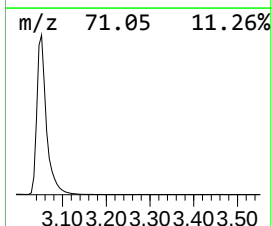
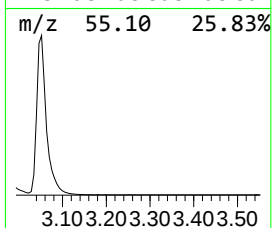
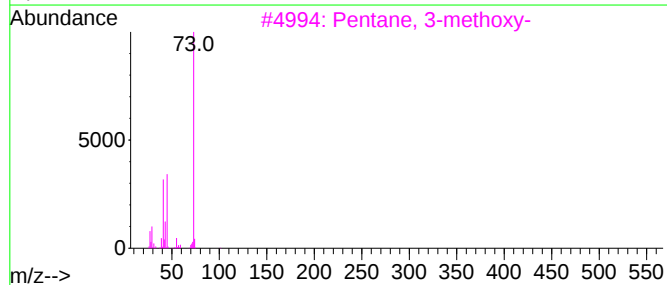
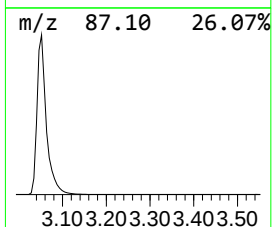
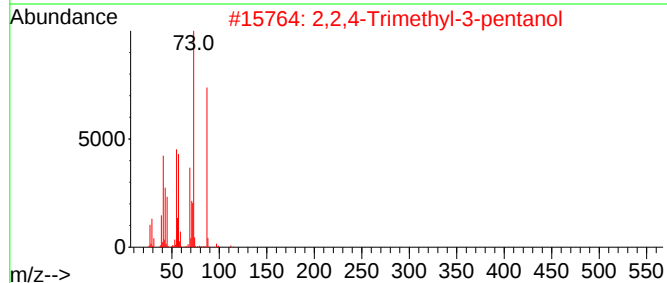
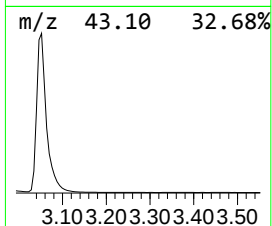
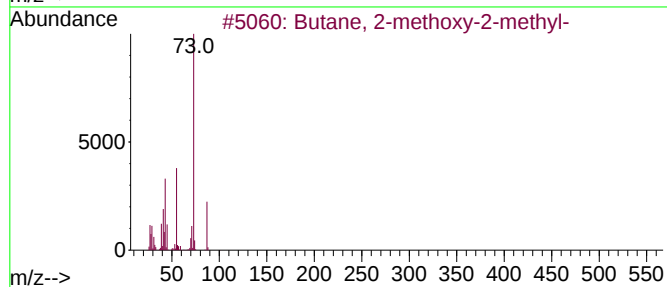
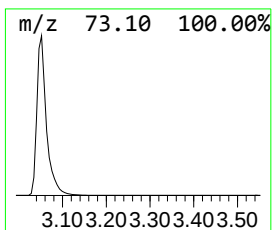
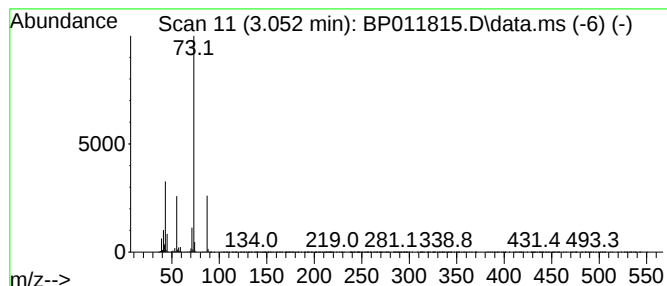
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.052	118.48 ng	14161500	1,4-Dichlorobenzene-d4	7.911

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011815.D
Acq On : 27 Sep 2022 14:50
Operator : CG/JU
Sample : N4835-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
529317-4

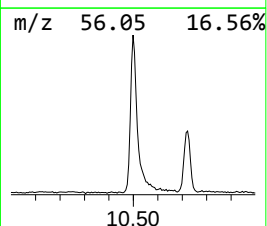
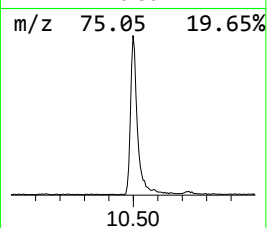
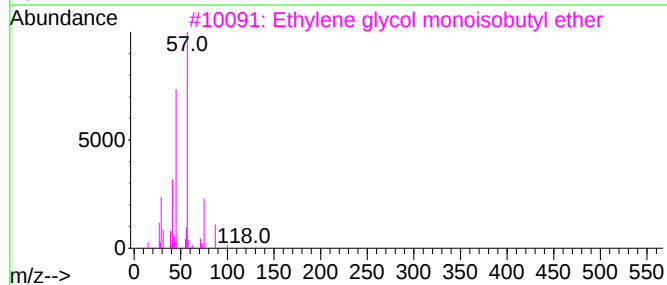
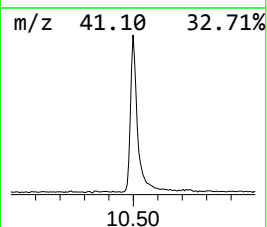
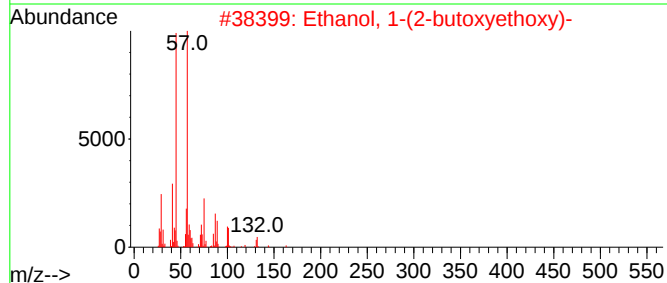
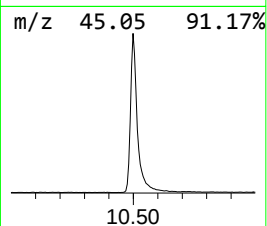
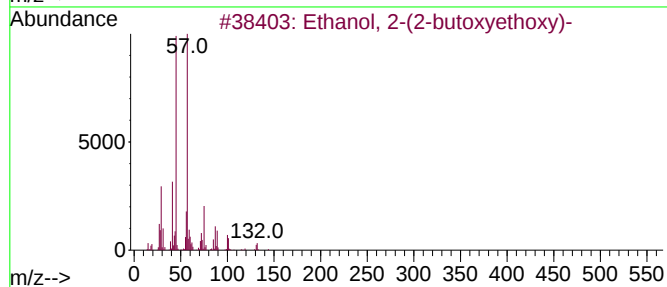
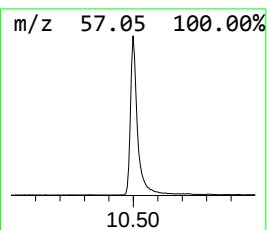
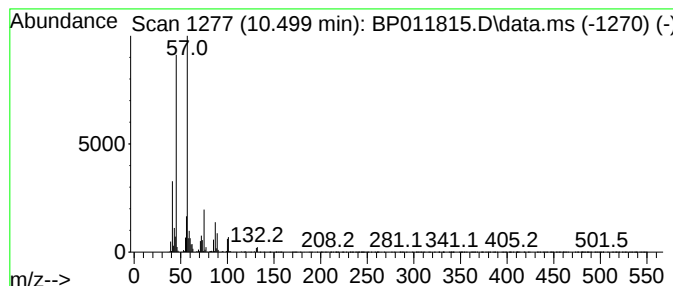
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.499	8.03 ng	1415250	Naphthalene-d8	10.722

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			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011815.D
Acq On : 27 Sep 2022 14:50
Operator : CG/JU
Sample : N4835-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
529317-4

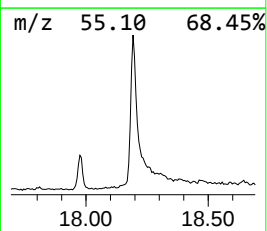
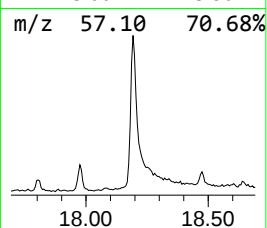
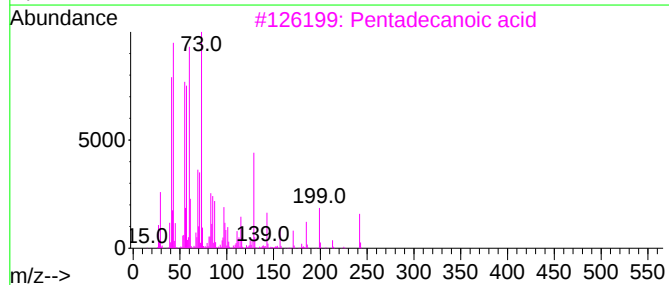
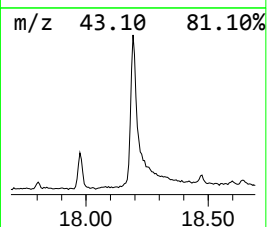
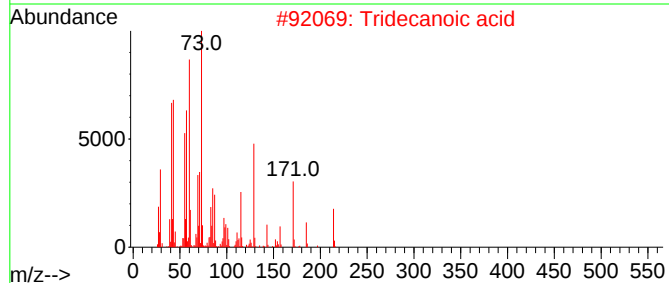
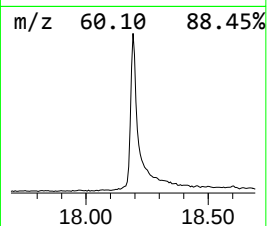
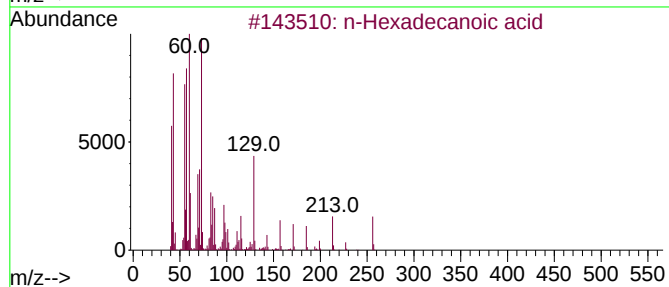
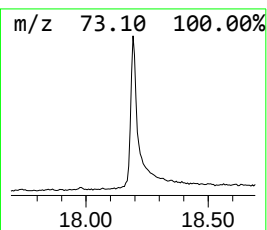
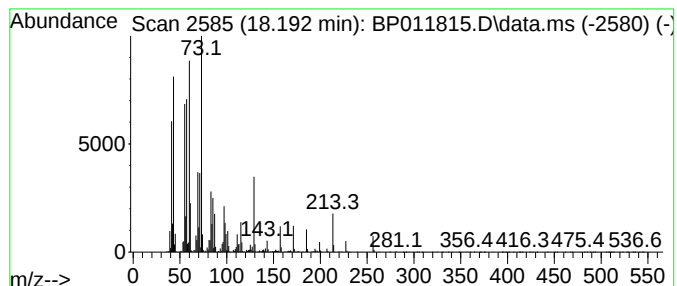
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	6.62 ng	1999980	Phenanthrene-d10	17.310

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	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Dodecanoic acid	200	C12H24O2	000143-07-7	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011815.D
Acq On : 27 Sep 2022 14:50
Operator : CG/JU
Sample : N4835-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
529317-4

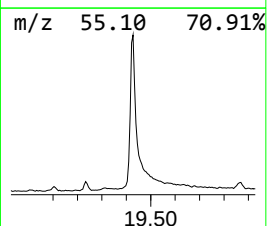
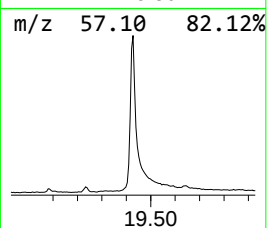
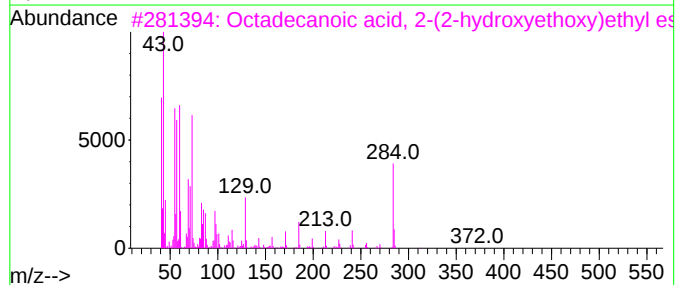
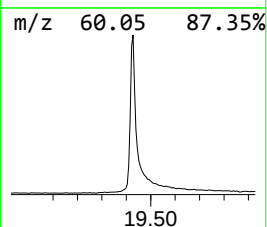
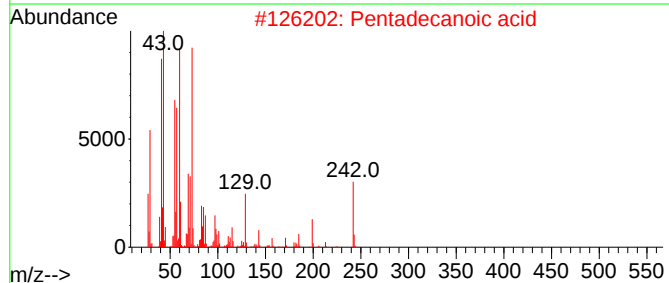
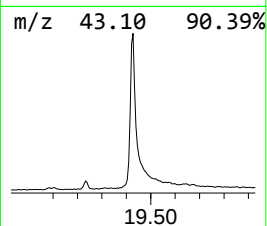
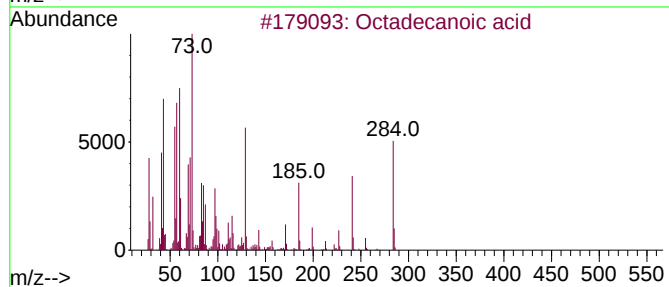
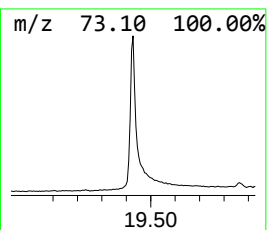
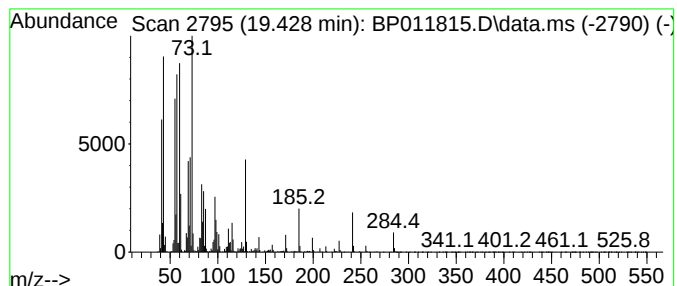
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
19.428	15.38 ng	4991150	Chrysene-d12	21.392

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	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011815.D
Acq On : 27 Sep 2022 14:50
Operator : CG/JU
Sample : N4835-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
529317-4

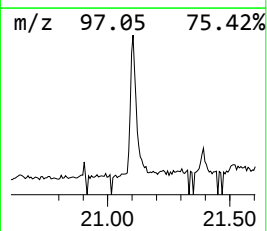
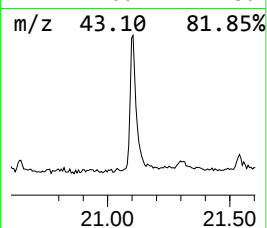
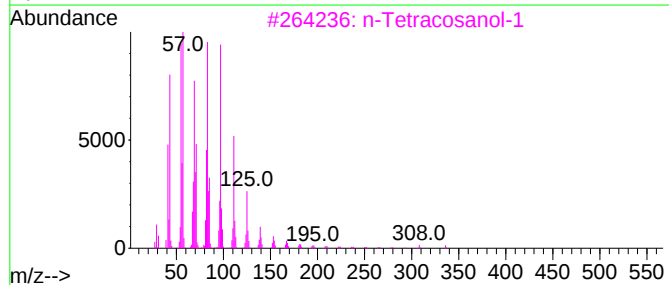
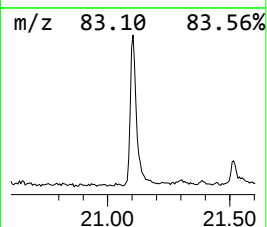
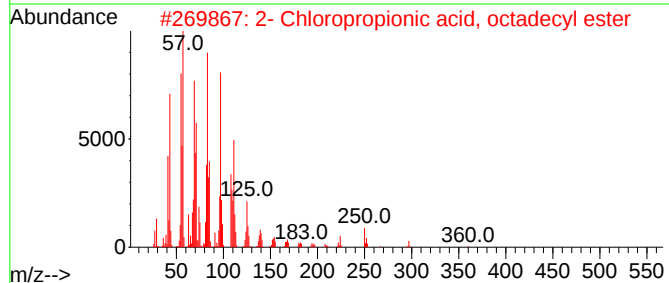
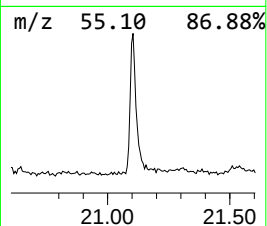
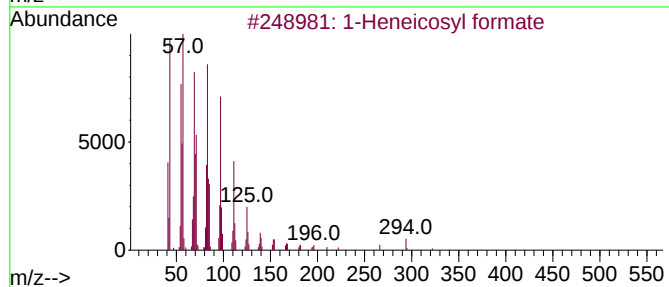
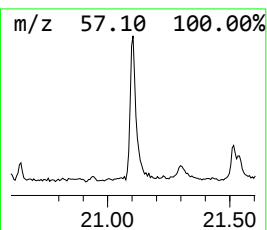
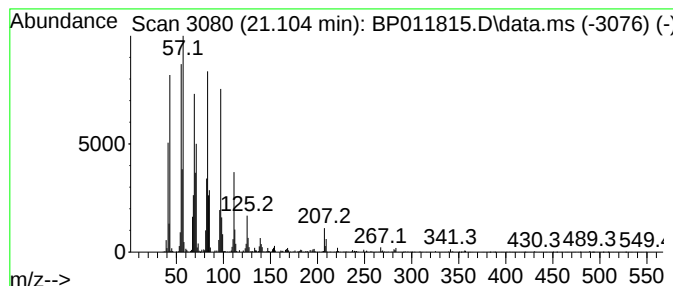
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosyl formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.104	2.52 ng	818188	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5			Cyclopentadecane	210	C15H30	000295-48-7	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011815.D
Acq On : 27 Sep 2022 14:50
Operator : CG/JU
Sample : N4835-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
529317-4

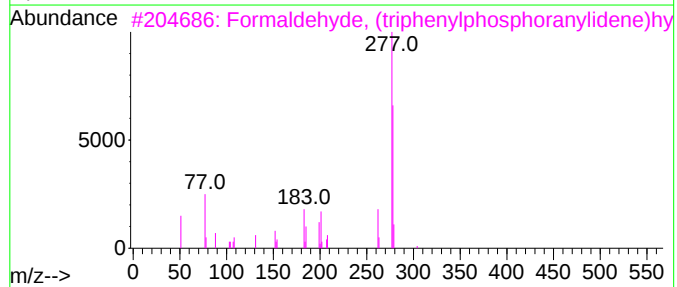
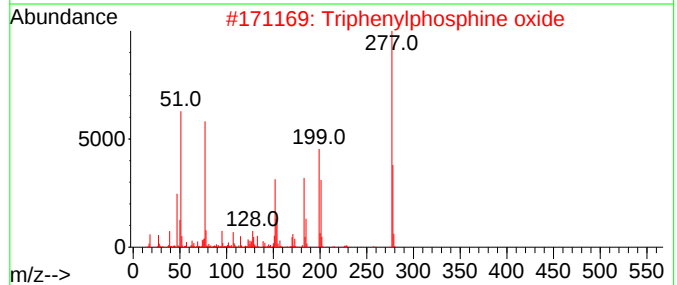
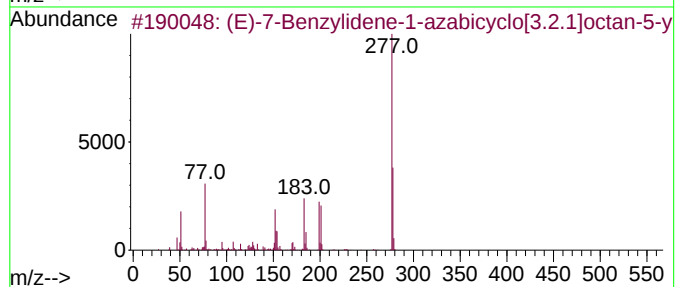
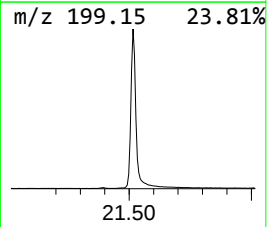
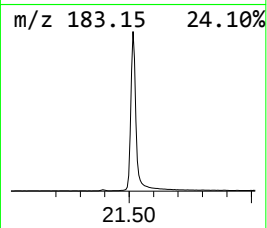
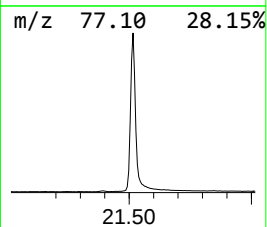
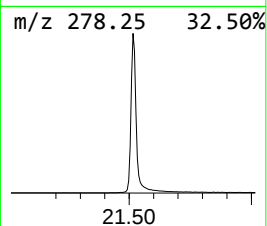
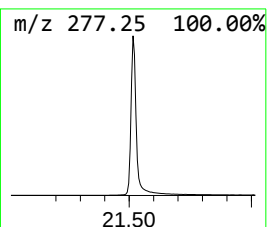
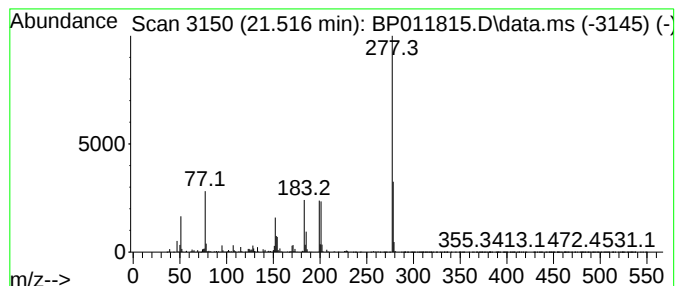
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 (E)-7-Benzylidene-1-azabicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.516	31.27 ng	10146200	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	94		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	92		
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64		
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43		
5	Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011815.D
Acq On : 27 Sep 2022 14:50
Operator : CG/JU
Sample : N4835-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
529317-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.052	118.5	ng	14161500	1	7.911	2390460	20.0
Ethanol, 2-(2-b...	10.499	8.0	ng	1415250	2	10.722	3526110	20.0
n-Hexadecanoic ...	18.192	6.6	ng	1999980	4	17.310	6041950	20.0
Octadecanoic acid	19.428	15.4	ng	4991150	5	21.392	6490130	20.0
1-Heneicosyl fo...	21.104	2.5	ng	818188	5	21.392	6490130	20.0
(E)-7-Benzylide...	21.516	31.3	ng	10146200	5	21.392	6490130	20.0