

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092322\
 Data File : BP011781.D
 Acq On : 23 Sep 2022 12:21
 Operator : CG/JU
 Sample : N4609-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DSN001

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: BP011781.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	7	11	27	rVB	871088	1373786	4.06%	1.993%
2	5.475	418	423	436	rVB	608958	978812	2.89%	1.420%
3	7.075	689	695	707	rVB	476805	798595	2.36%	1.159%
4	9.081	1030	1036	1047	rVB	912059	1497073	4.42%	2.172%
5	10.728	1309	1316	1331	rVB	319209	565923	1.67%	0.821%
6	13.186	1725	1734	1745	rBV	2262681	3295317	9.74%	4.781%
7	14.563	1957	1968	1974	rBV	557682	852409	2.52%	1.237%
8	16.051	2215	2221	2230	rBV	1948152	2741589	8.10%	3.977%
9	17.245	2418	2424	2431	rBV	341165	565791	1.67%	0.821%
10	17.316	2431	2436	2449	rVB	873229	1278755	3.78%	1.855%
11	18.198	2582	2586	2590	rBV	346497	471539	1.39%	0.684%
12	18.245	2590	2594	2603	rVB2	301476	519628	1.54%	0.754%
13	18.657	2659	2664	2674	rBV	915102	1334354	3.94%	1.936%
14	19.374	2781	2786	2793	rBV	5976880	6653089	19.66%	9.652%
15	19.874	2866	2871	2877	rBV	6965496	7959804	23.52%	11.548%
16	21.404	3126	3131	3137	rBV	1436647	1934700	5.72%	2.807%
17	21.539	3147	3154	3186	rBV	19012595	33835805	100.00%	49.089%
18	23.851	3541	3547	3556	rVB2	1092650	2270876	6.71%	3.295%

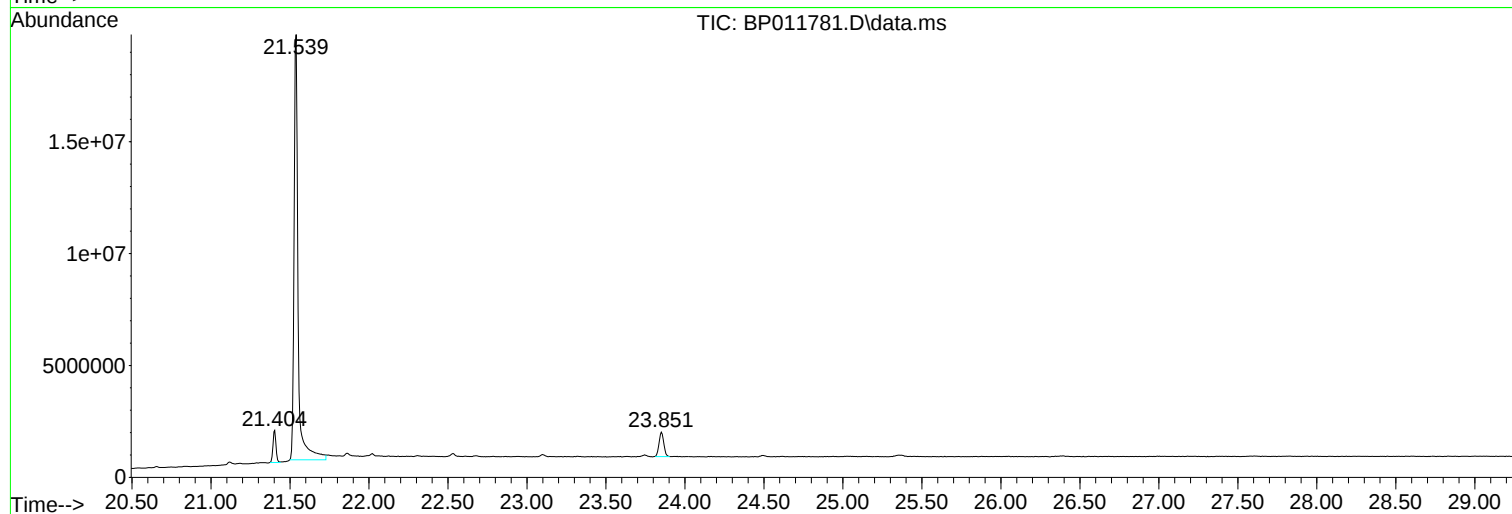
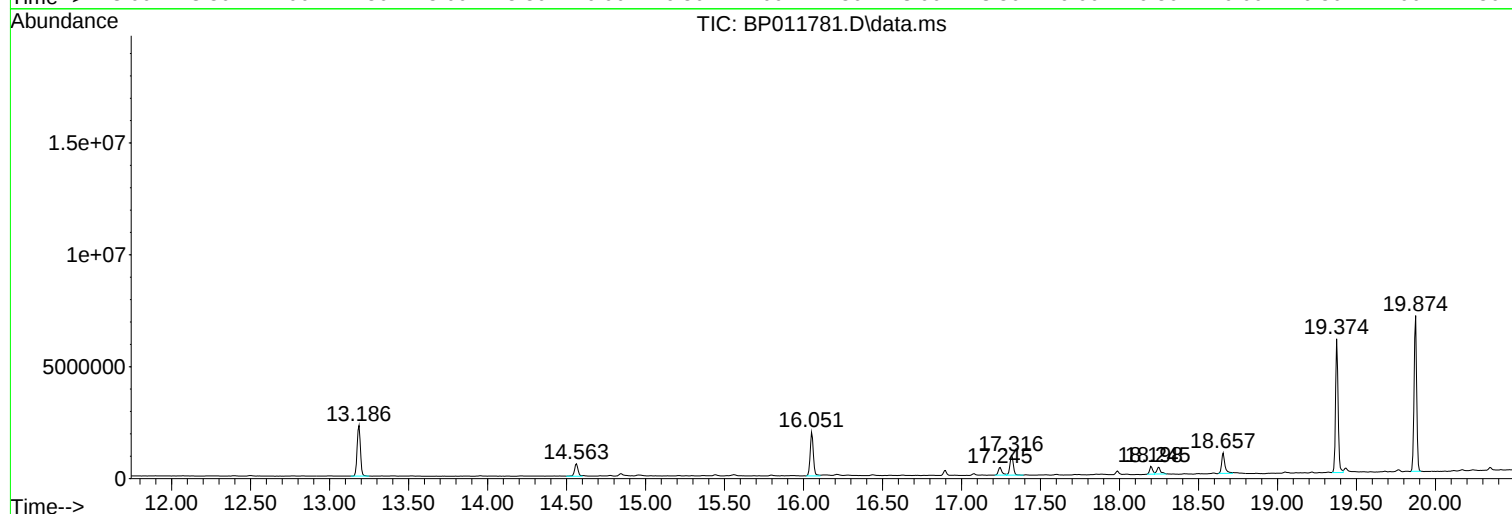
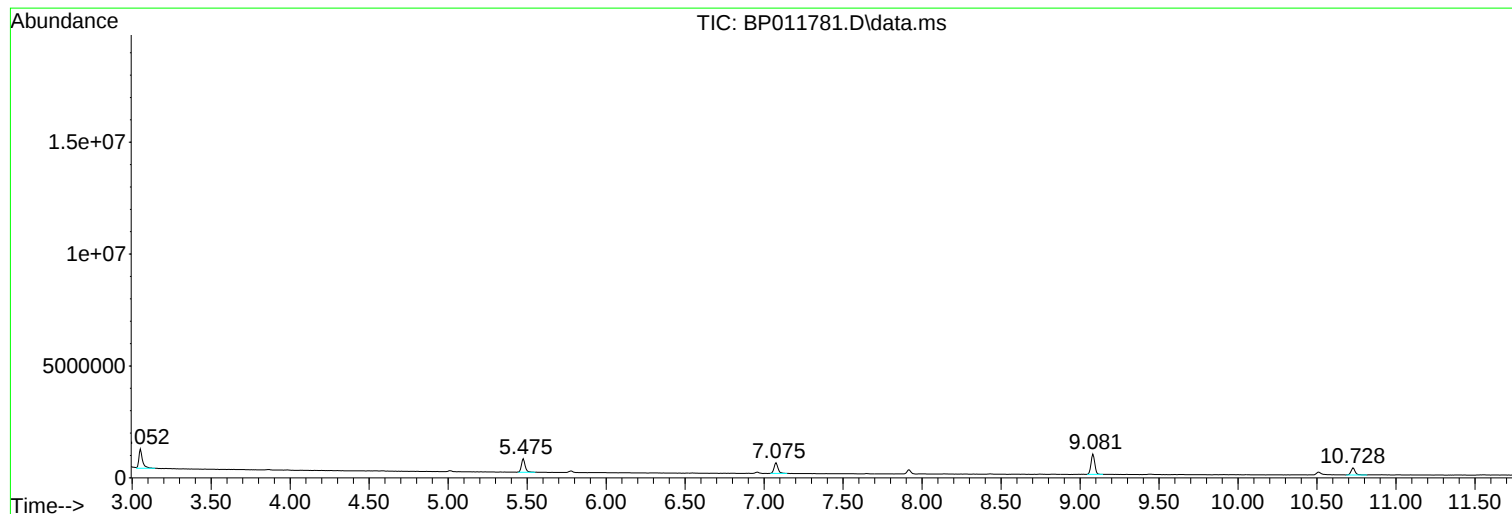
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
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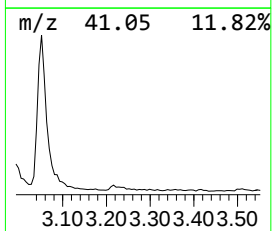
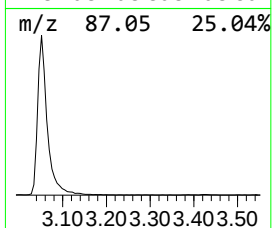
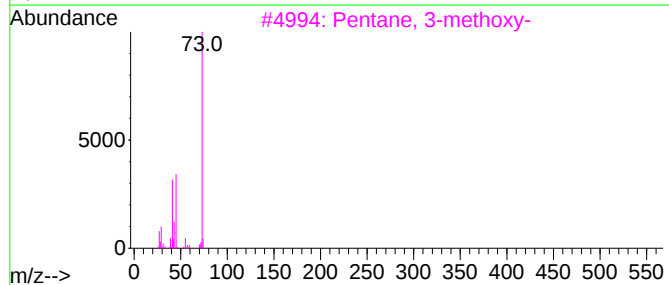
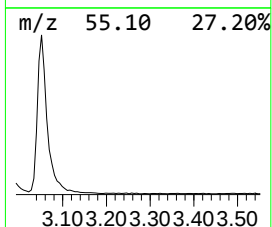
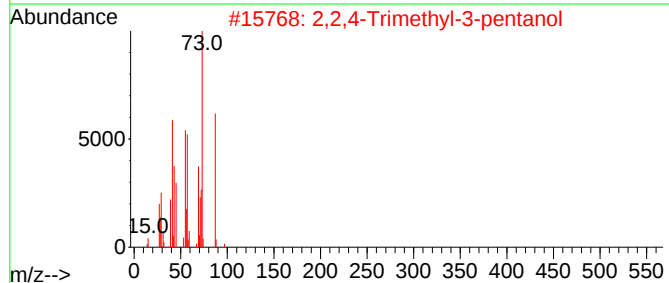
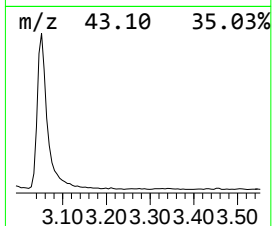
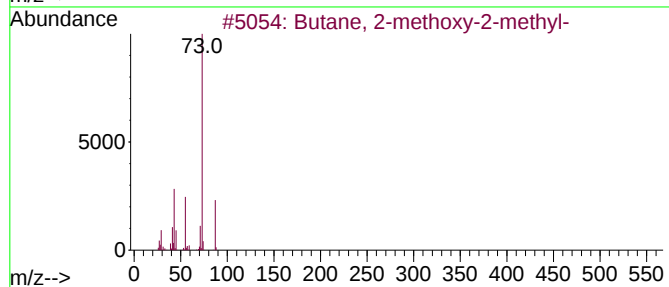
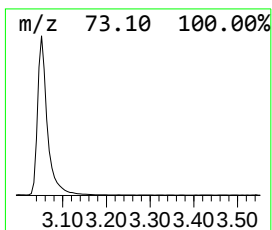
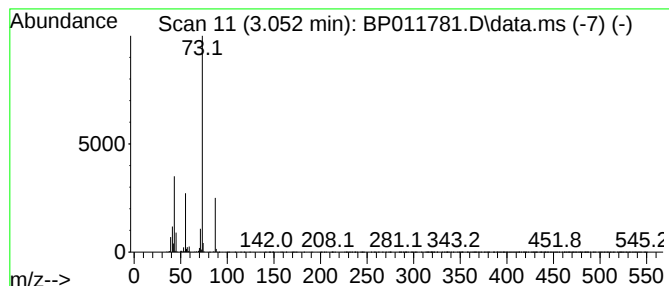
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.052	34.41 ng	1373790	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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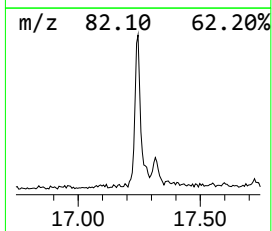
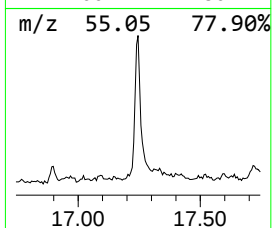
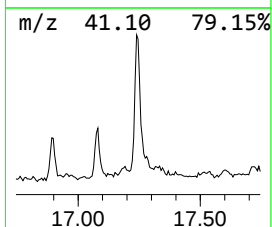
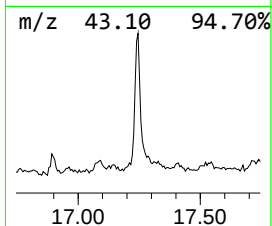
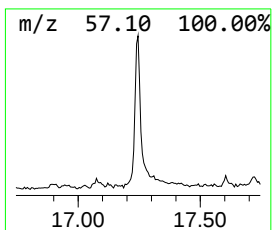
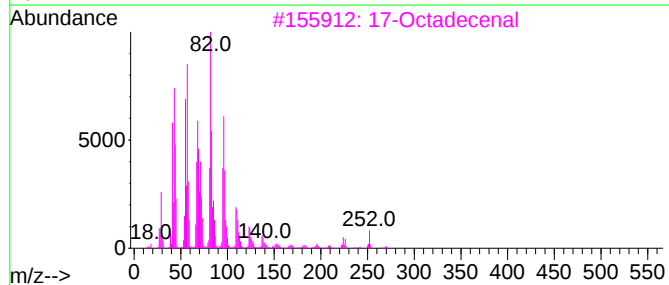
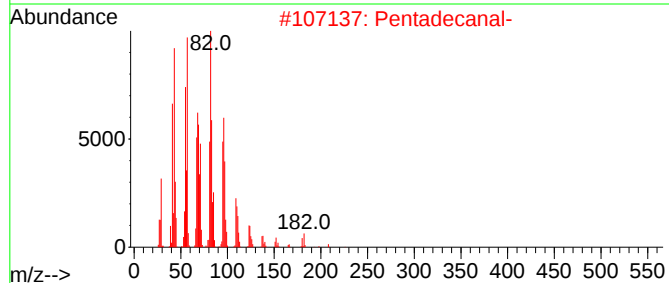
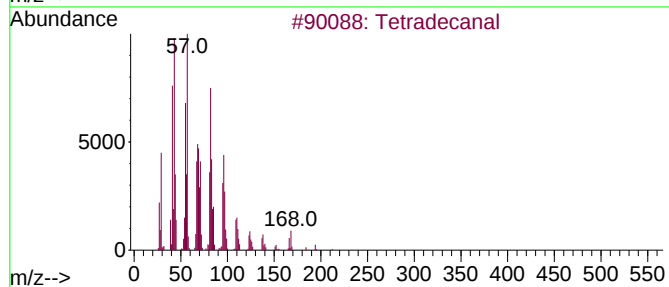
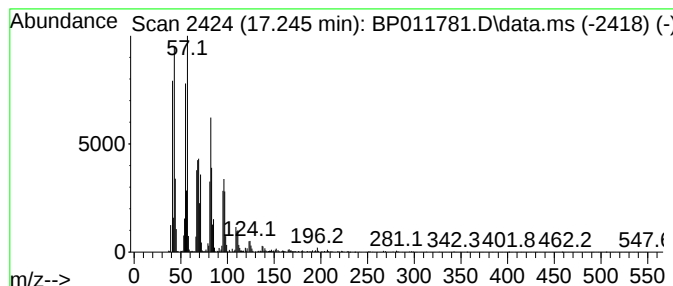
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Tetradecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.245	8.85 ng	565791	Phenanthrene-d10	17.316

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanal	212	C14H28O	000124-25-4	95
2		Pentadecanal-	226	C15H30O	002765-11-9	94
3		17-Octadecenal	266	C18H34O	056554-86-0	91
4		Octadecanal	268	C18H36O	000638-66-4	91
5		E-2-Tetradecen-1-ol	212	C14H28O	1000130-83-7	91



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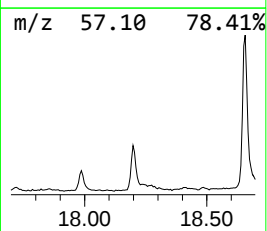
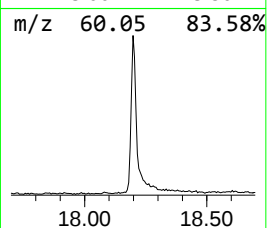
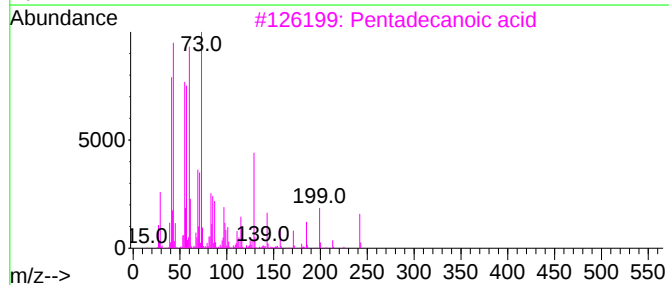
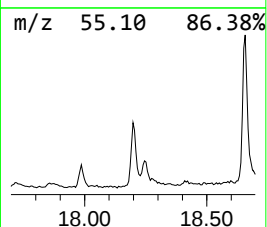
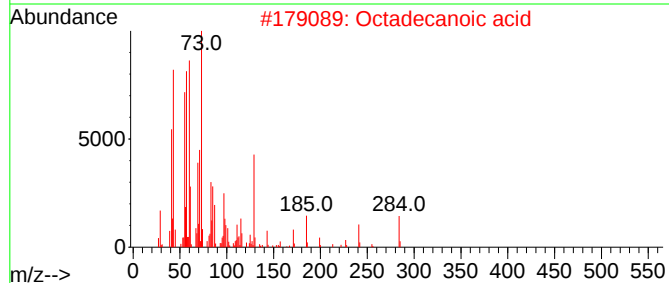
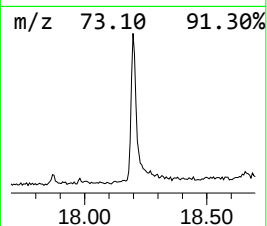
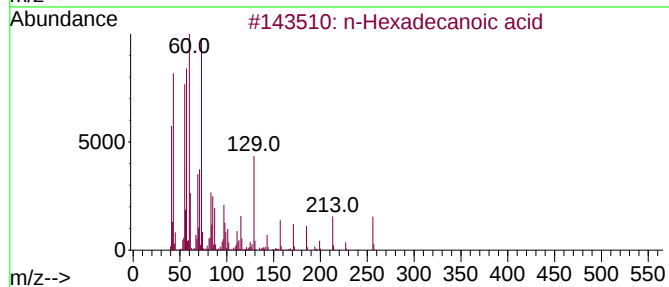
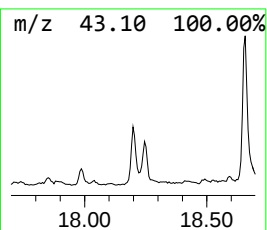
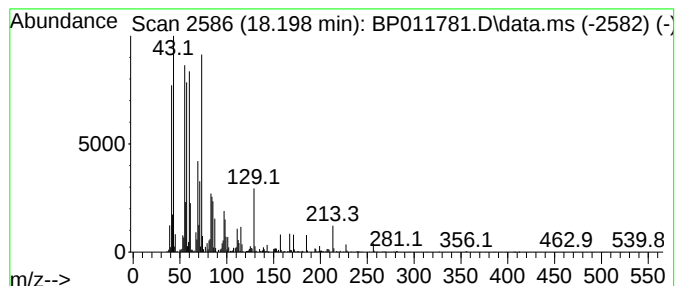
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.198	7.37 ng	471539	Phenanthrene-d10		17.316	
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	83
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
5	Tridecanoic acid		214	C13H26O2	000638-53-9	80



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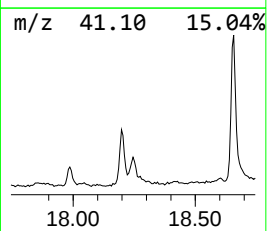
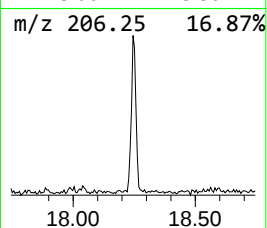
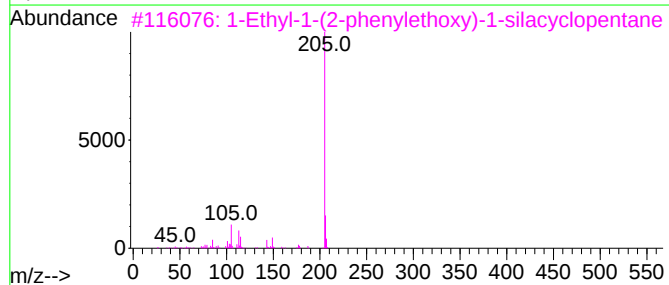
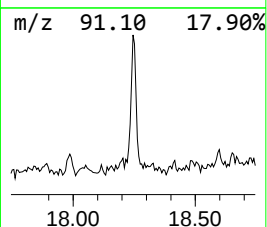
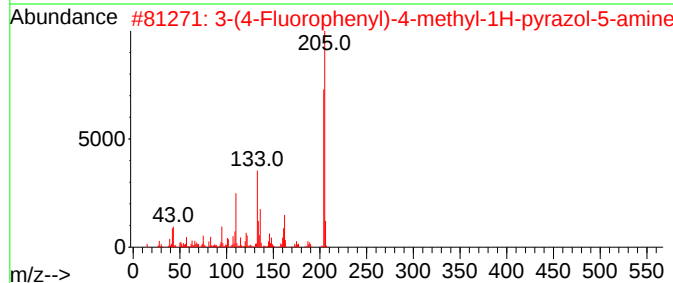
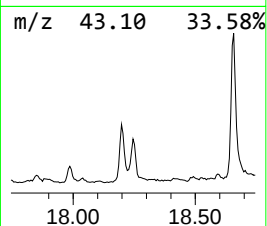
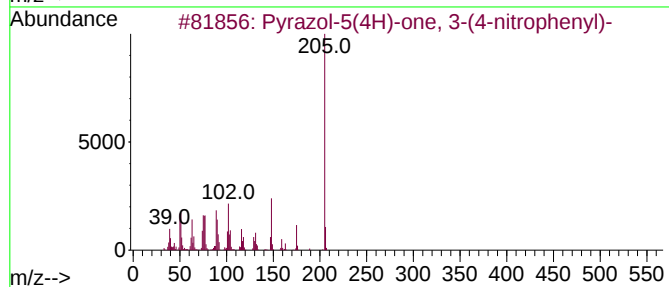
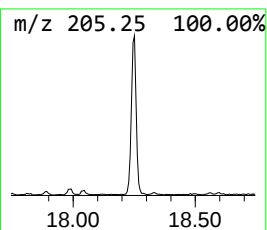
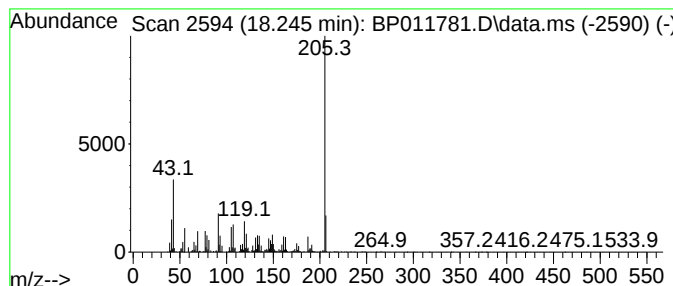
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Peak Number 4 Pyrazol-5(4H)-one, 3-(4-nit... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.245	8.13 ng	519628	Phenanthrene-d10	17.316	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazol-5(4H)-one, 3-(4-nitrophe...	205	C9H7N3O3	054945-13-0	58
2	3-(4-Fluorophenyl)-4-methyl-1H-p...	205	C11H12FN3	1000509-34-4	53
3	1-Ethyl-1-(2-phenylethoxy)-1-sil...	234	C14H22OSi	1000279-36-8	50
4	1,3-Benzenedicarboxylic acid, bi...	278	C14H14O6	007195-43-9	50
5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	45



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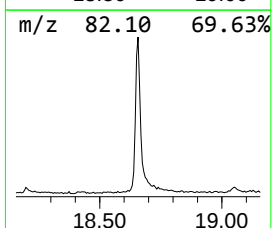
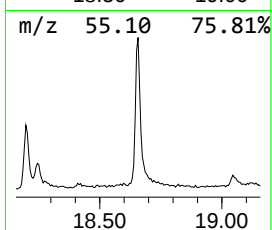
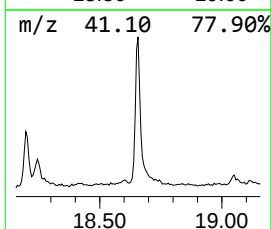
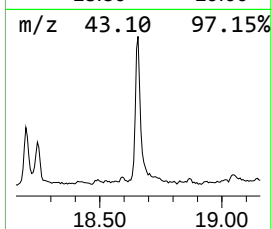
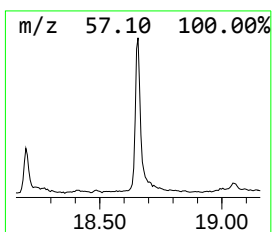
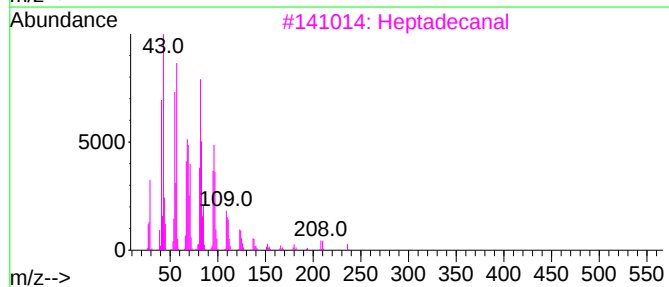
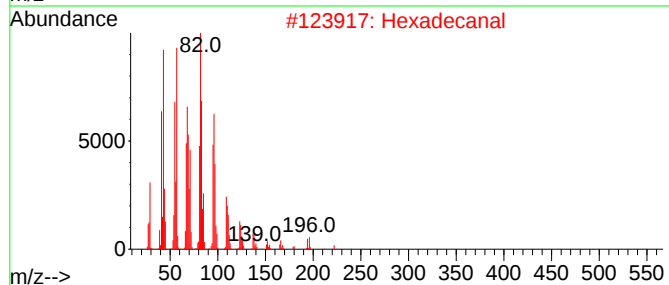
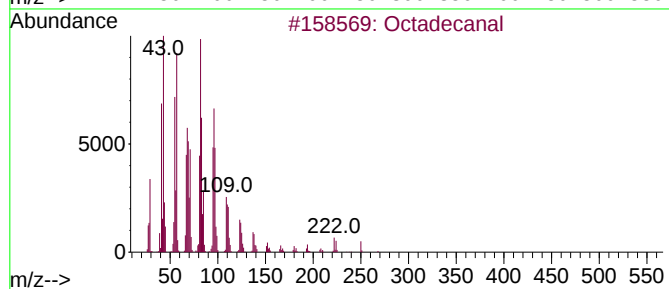
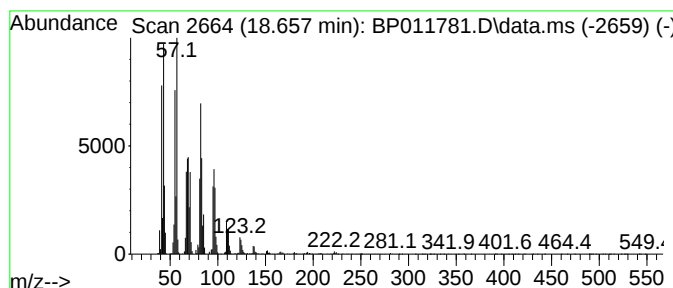
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.657	20.87 ng	1334350	Phenanthrene-d10	17.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	99
2			Hexadecanal	240	C16H32O	000629-80-1	96
3			Heptadecanal	254	C17H34O	1000376-70-0	95
4			Pentadecanal-	226	C15H30O	002765-11-9	94
5			9-Octadecen-1-ol, (Z)-	268	C18H36O	000143-28-2	93



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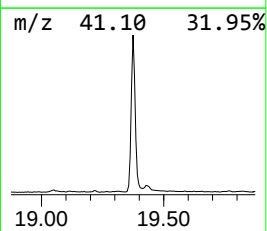
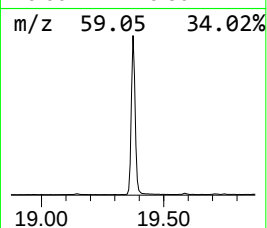
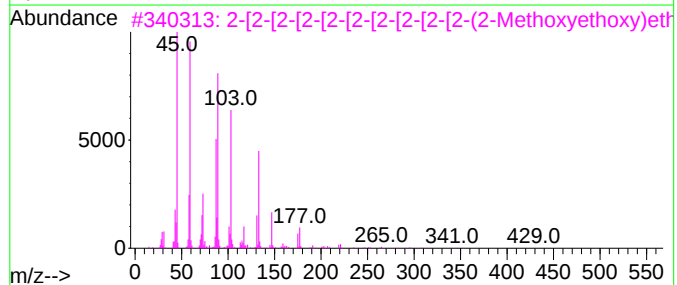
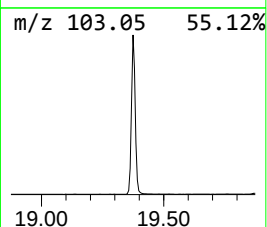
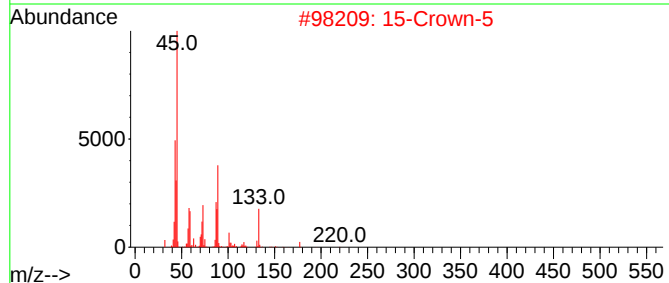
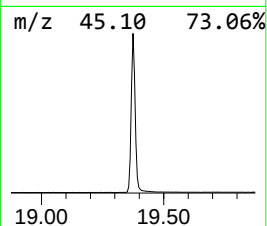
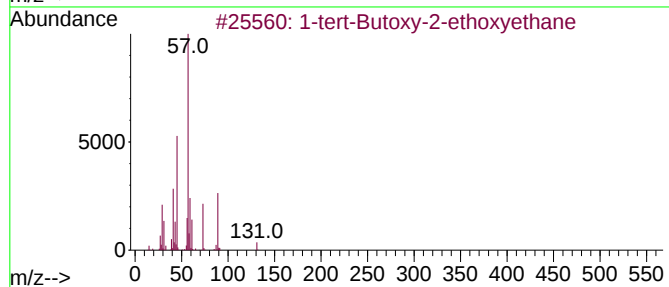
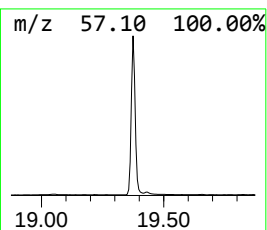
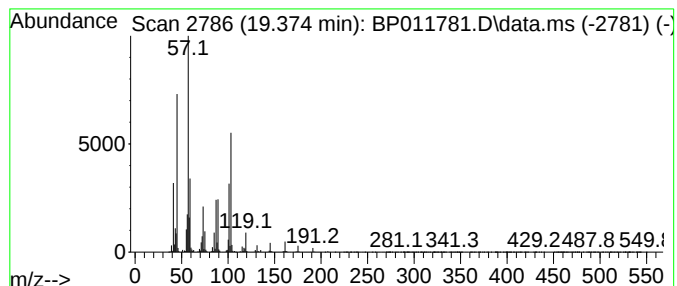
Instrument :
BNA_P
ClientSampleId :
DSN001

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 unknown19.374 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.374	68.78 ng	6653090	Chrysene-d12		21.404	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-tert-Butoxy-2-ethoxyethane		146	C8H18O2	051422-54-9	43
2	15-Crown-5		220	C10H20O5	033100-27-5	35
3	2-[2-[2-[2-[2-[2-[2-[2-(2-...		516	C23H48O12	1010352-04-4	27
4	2-[2-[2-[2-[2-[2-(2-Methoxyet...		384	C17H36O9	025990-96-9	27
5	2-[2-[2-[2-[2-[2-(2-Methox...		428	C19H40O10	006048-68-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092322\
Data File : BP011781.D
Acq On : 23 Sep 2022 12:21
Operator : CG/JU
Sample : N4609-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DSN001

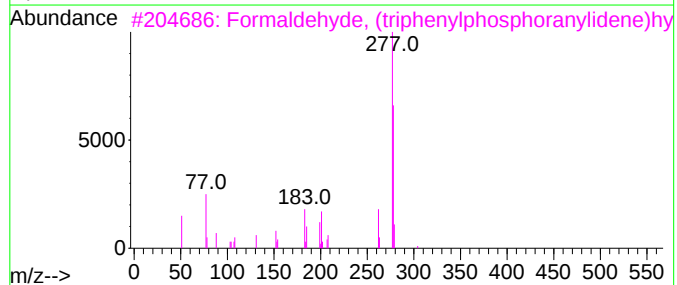
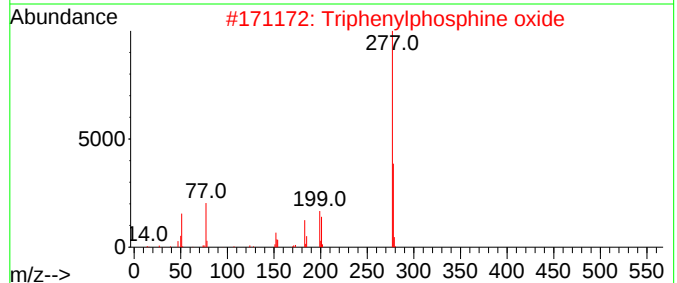
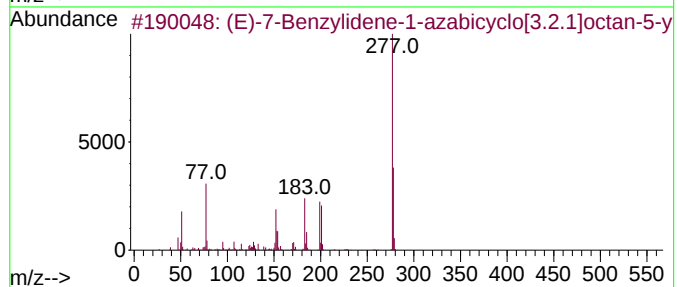
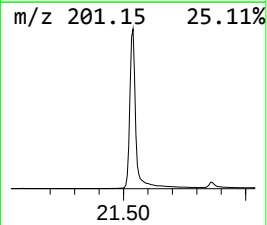
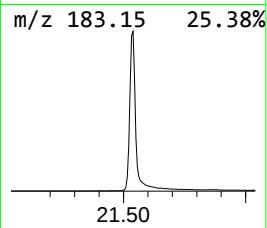
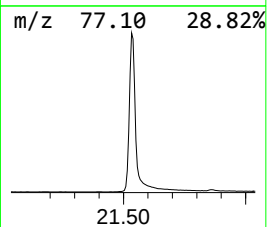
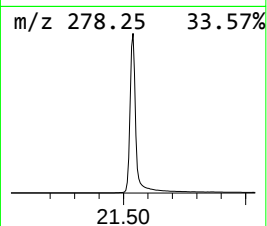
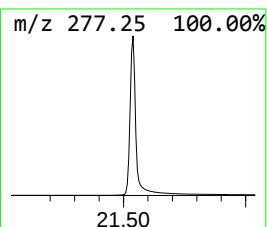
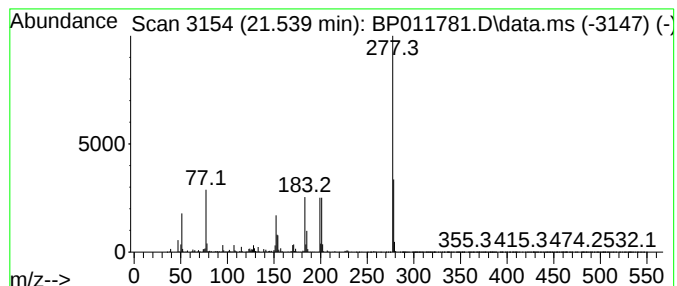
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.539	349.78 ng	33835800	Chrysene-d12	21.404

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	93		
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45		
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\BP092322\
Data File : BP011781.D
Acq On : 23 Sep 2022 12:21
Operator : CG/JU
Sample : N4609-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DSN001

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.052	34.4	ng	1373790	1	7.916	798595	20.0
Tetradecanal	17.245	8.8	ng	565791	4	17.316	1278760	20.0
n-Hexadecanoic ...	18.198	7.4	ng	471539	4	17.316	1278760	20.0
Pyrazol-5(4H)-o...	18.245	8.1	ng	519628	4	17.316	1278760	20.0
Octadecanal	18.657	20.9	ng	1334350	4	17.316	1278760	20.0
unknown19.374	19.374	68.8	ng	6653090	5	21.404	1934700	20.0
(E)-7-Benzylide...	21.539	349.8	ng	33835800	5	21.404	1934700	20.0