

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020822\
 Data File : BP009063.D
 Acq On : 08 Feb 2022 17:45
 Operator : CG/JU
 Sample : N1421-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-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-BP020722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009063.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.017	3	5	14	rVB	285931	290239	3.71%	0.535%
2	5.393	403	409	431	rBV	2188028	3447893	44.12%	6.351%
3	6.987	671	680	711	rBV	1997744	3630308	46.45%	6.687%
4	7.804	811	819	829	rBV	645207	1079976	13.82%	1.989%
5	8.963	1008	1016	1039	rBV	1446051	2642806	33.82%	4.868%
6	10.604	1287	1295	1312	rBV	742112	1386927	17.75%	2.555%
7	13.069	1706	1714	1729	rBV	3807927	5783689	74.01%	10.654%
8	14.445	1941	1948	1966	rBV	1011735	1613741	20.65%	2.973%
9	15.945	2196	2203	2222	rBV	2420561	3943433	50.46%	7.264%
10	17.204	2411	2417	2430	rBV	1073108	1651443	21.13%	3.042%
11	17.992	2546	2551	2556	rBV2	71358	150186	1.92%	0.277%
12	18.045	2556	2560	2566	rVV	227241	401525	5.14%	0.740%
13	18.104	2566	2570	2593	rVB	1135852	1972006	25.23%	3.633%
14	19.027	2722	2727	2736	rVB	942560	1126615	14.42%	2.075%
15	19.227	2751	2761	2777	rBV	3082941	7815211	100.00%	14.396%
16	19.339	2777	2780	2794	rVB	463703	909053	11.63%	1.675%
17	19.692	2836	2840	2847	rBV2	92342	166823	2.13%	0.307%
18	19.769	2848	2853	2860	rVB	4922223	6156124	78.77%	11.340%
19	20.045	2896	2900	2903	rBV	161848	201034	2.57%	0.370%
20	20.074	2903	2905	2914	rVB4	107485	149387	1.91%	0.275%
21	20.233	2928	2932	2940	rBV	961805	1295719	16.58%	2.387%
22	20.398	2954	2960	2963	rBV2	742978	970687	12.42%	1.788%
23	20.439	2963	2967	2974	rVB	700075	986310	12.62%	1.817%
24	21.010	3061	3064	3071	rBV3	293237	385166	4.93%	0.709%
25	21.168	3088	3091	3096	rVB	114695	132050	1.69%	0.243%
26	21.298	3109	3113	3125	rBV	1602738	2114216	27.05%	3.894%
27	21.416	3128	3133	3144	rBV	731885	1247935	15.97%	2.299%
28	23.698	3515	3521	3528	rVB2	1296745	2637018	33.74%	4.858%

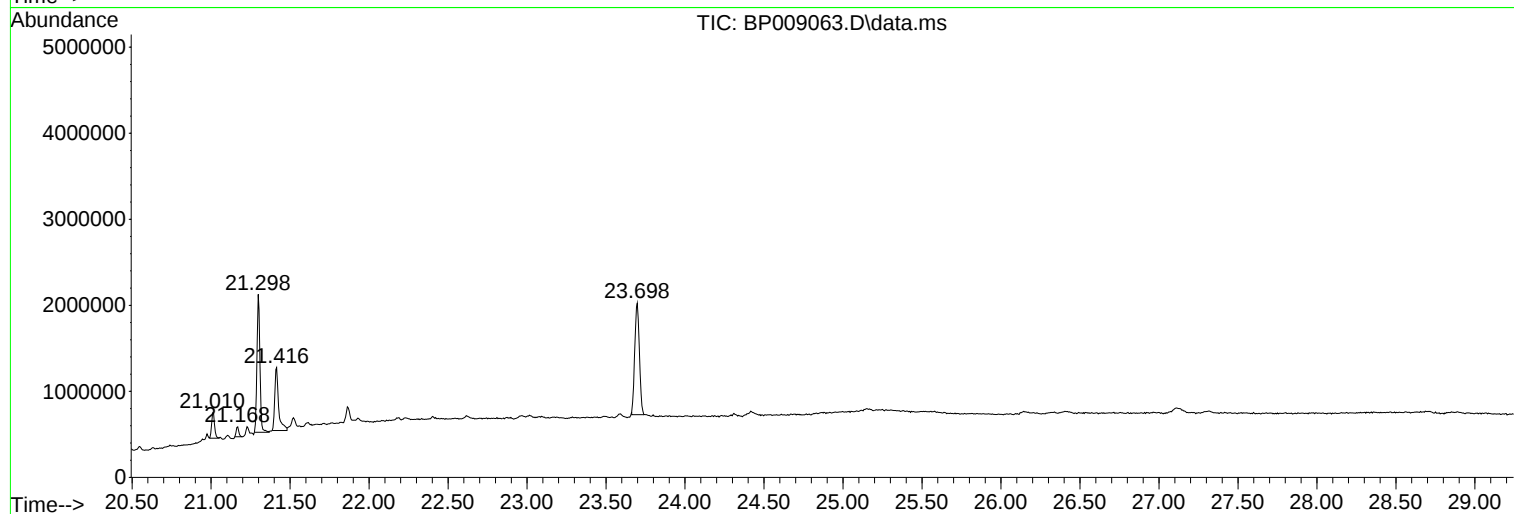
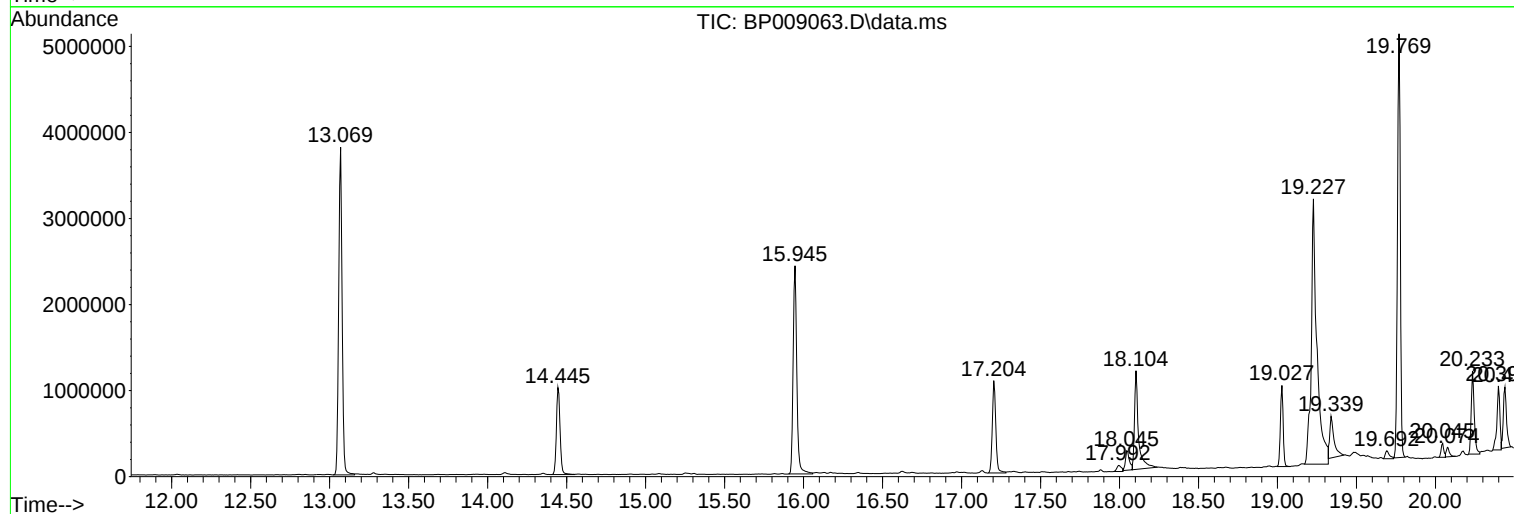
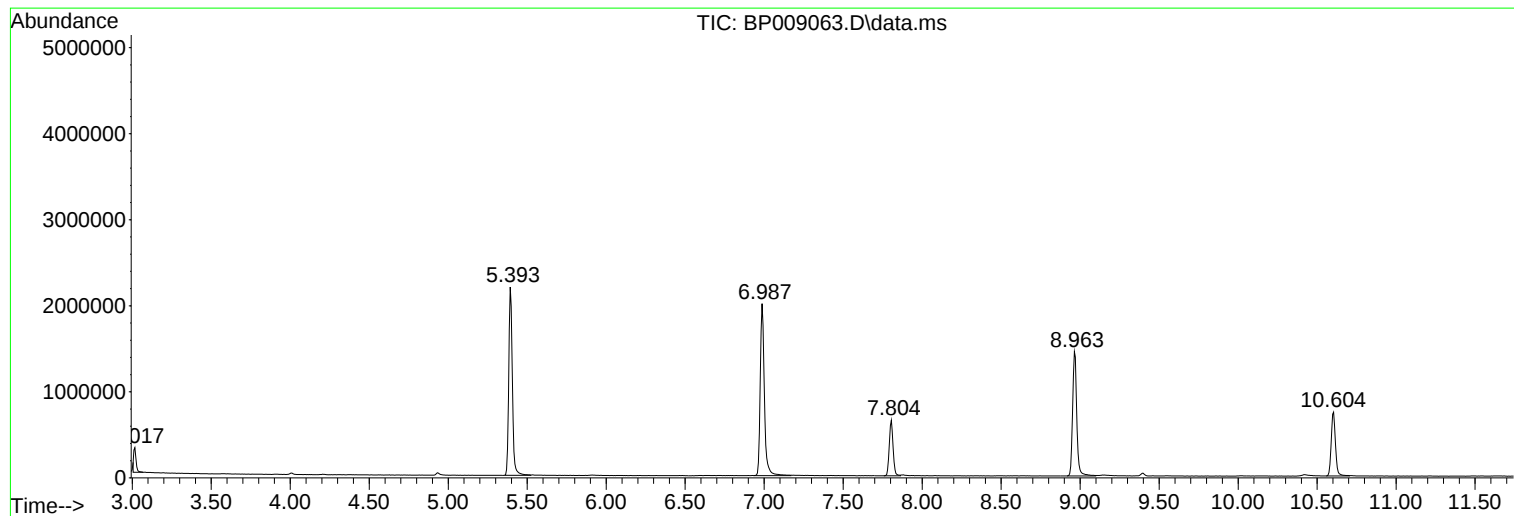
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
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Instrument :
BNA_P
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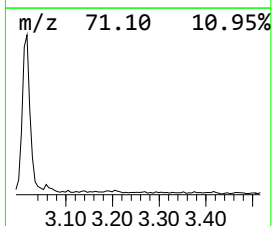
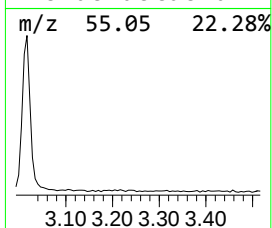
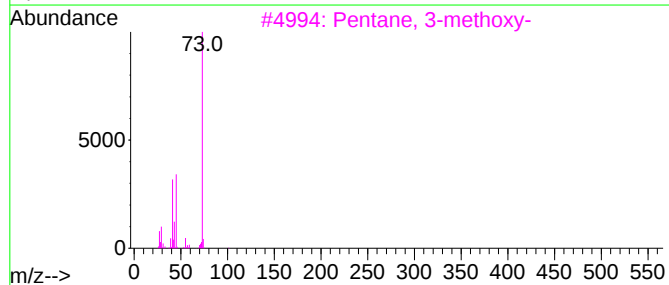
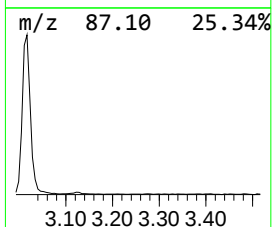
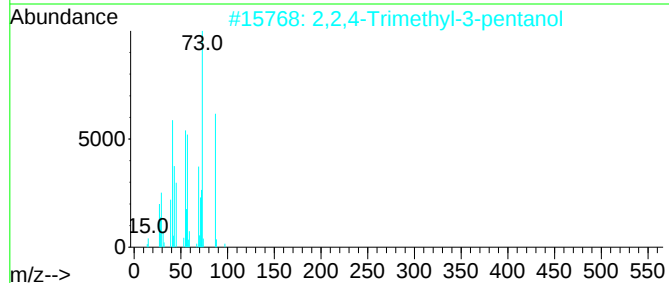
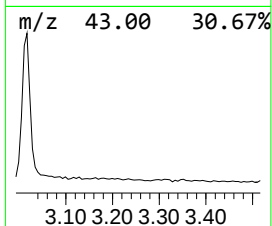
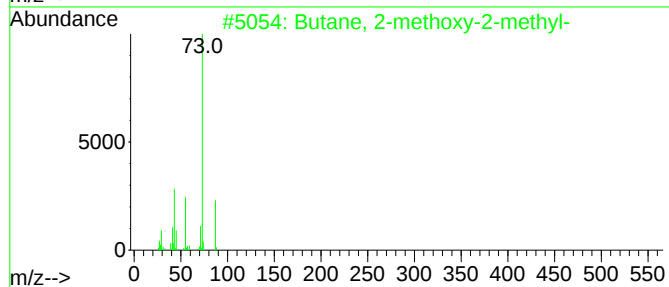
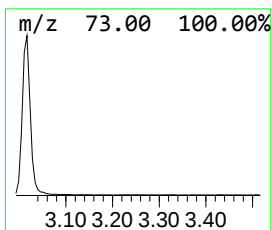
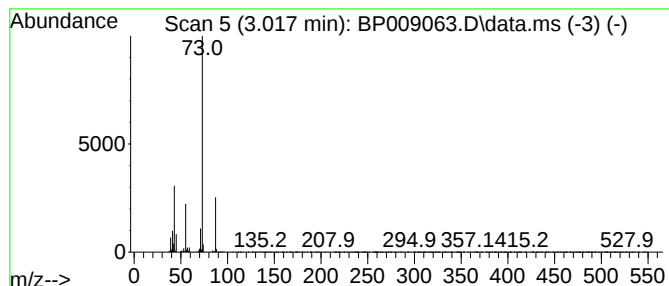
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.017	5.37 ng	290239	1,4-Dichlorobenzene-d4	7.804

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	56
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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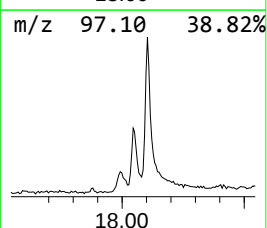
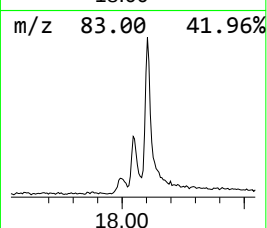
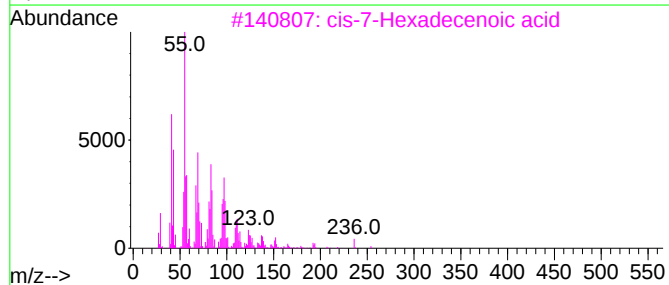
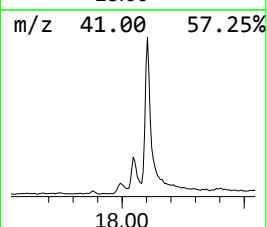
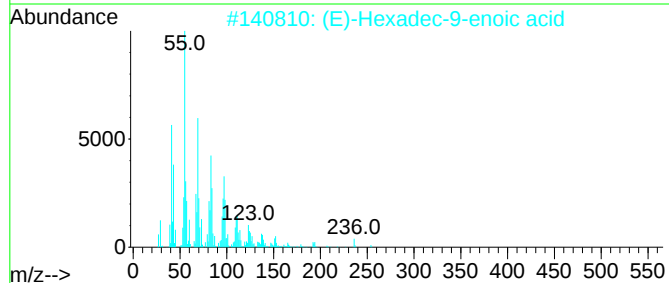
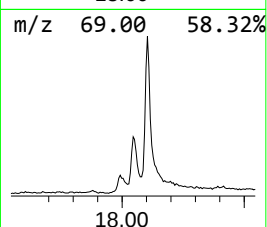
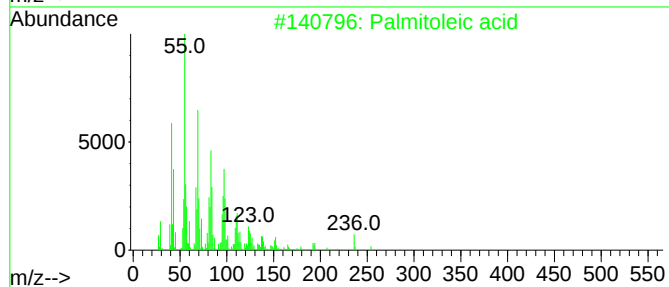
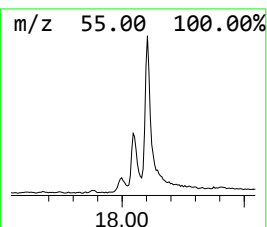
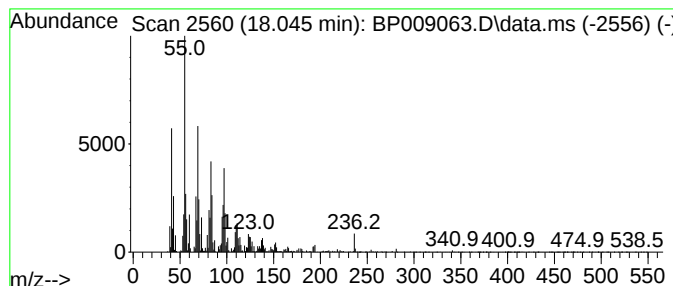
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Palmitoleic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.045	4.86 ng	401525	Phenanthrene-d10	17.204	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	98
2	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	98
3	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	97
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
5	n-Propyl 11-octadecenoate	324	C21H40O2	1000336-71-7	90



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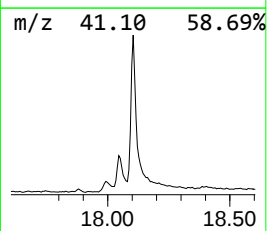
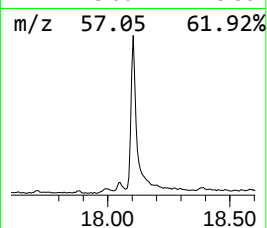
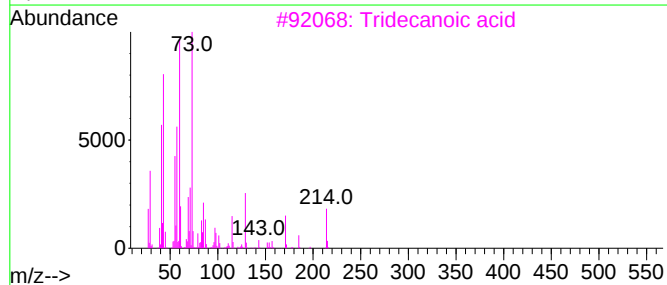
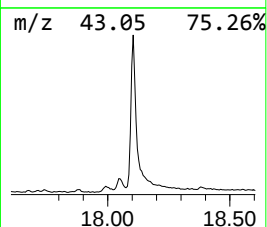
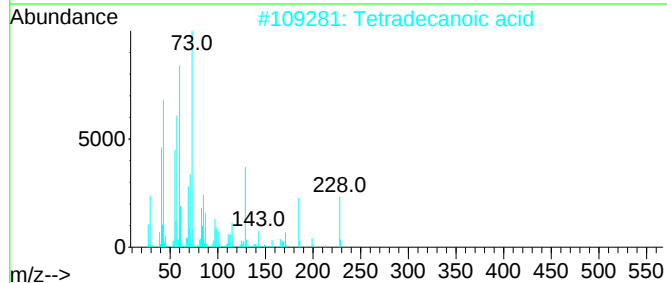
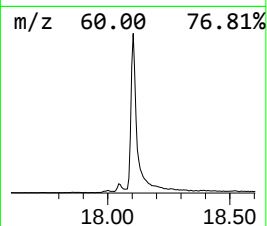
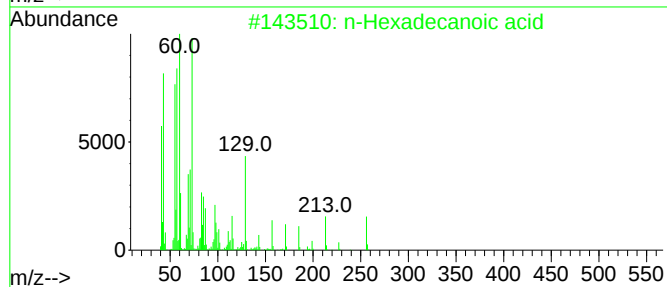
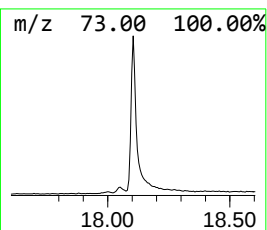
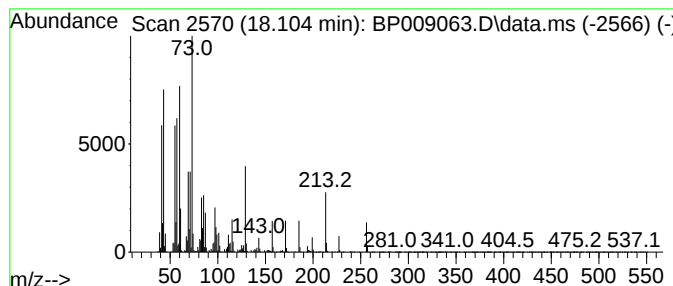
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BNA_P
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.104	23.88 ng	1972010	Phenanthrene-d10		17.204	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	94
3	Tridecanoic acid		214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
5	n-Decanoic acid		172	C10H20O2	000334-48-5	53



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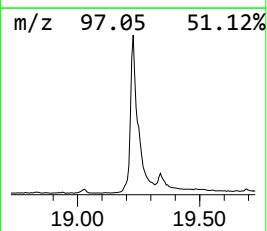
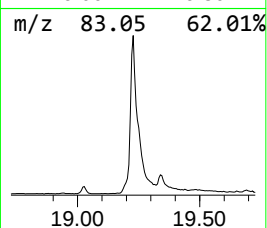
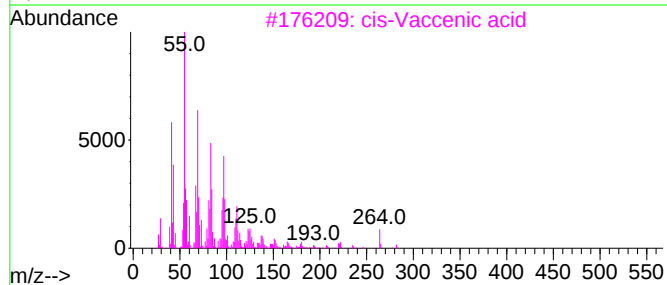
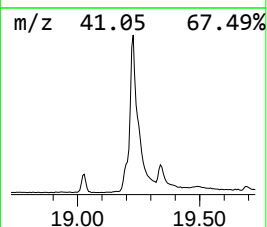
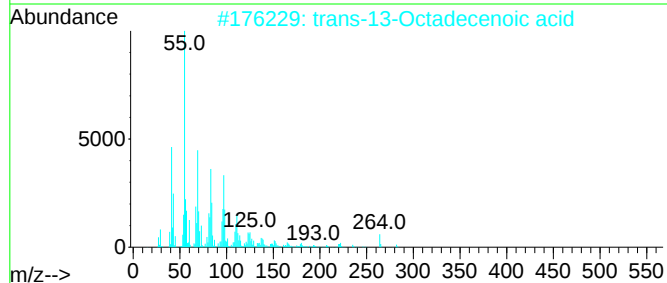
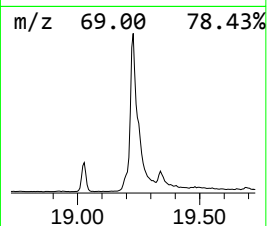
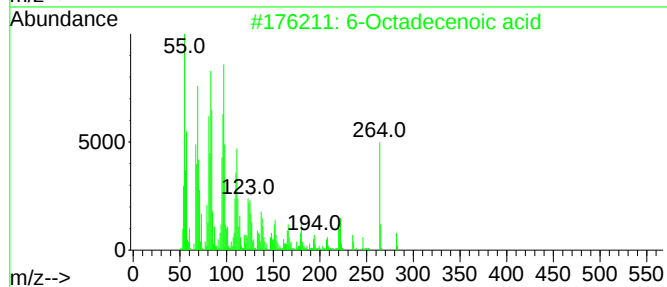
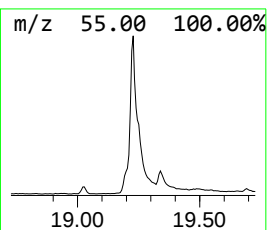
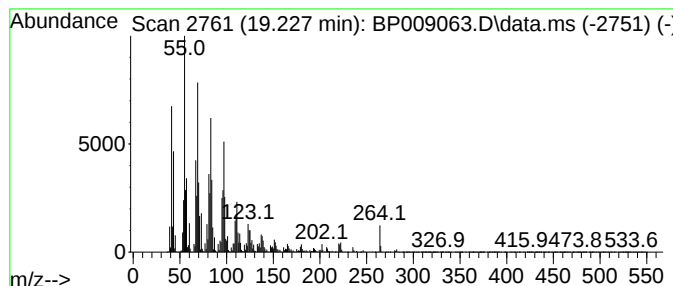
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Peak Number 5 6-Octadecenoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.227	94.65 ng	7815210	Phenanthrene-d10	17.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Octadecenoic acid	282	C18H34O2	1000336-66-8	95
2			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	94
3			cis-Vaccenic acid	282	C18H34O2	000506-17-2	93
4			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91
5			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	89



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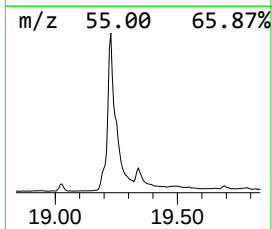
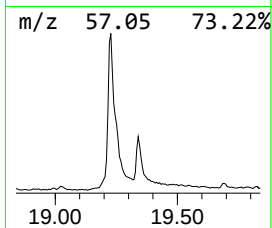
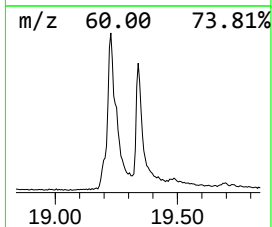
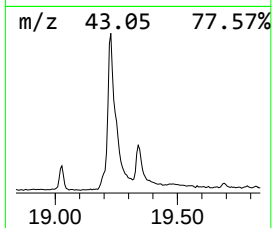
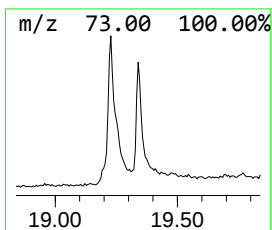
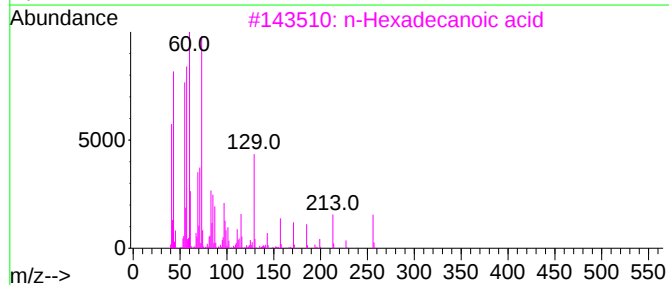
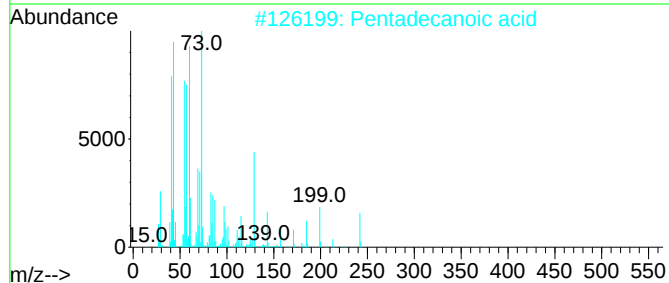
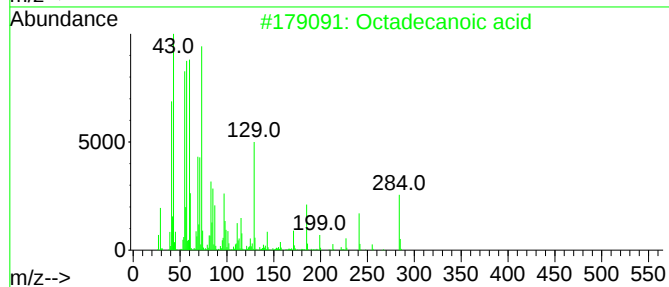
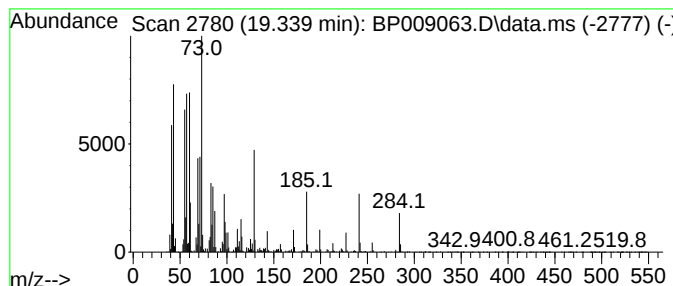
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	8.60 ng	909053	Chrysene-d12	21.298

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	87
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	58



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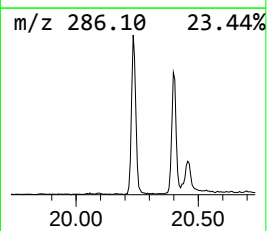
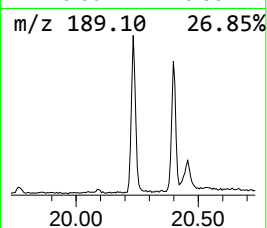
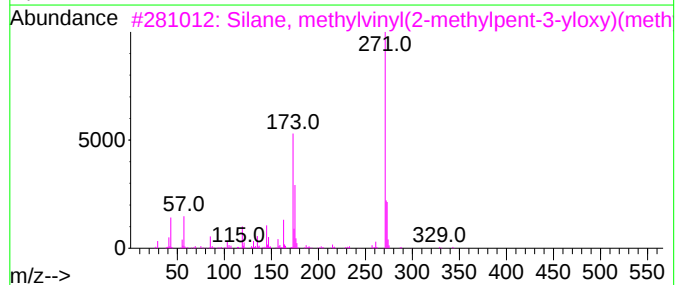
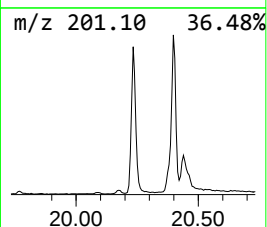
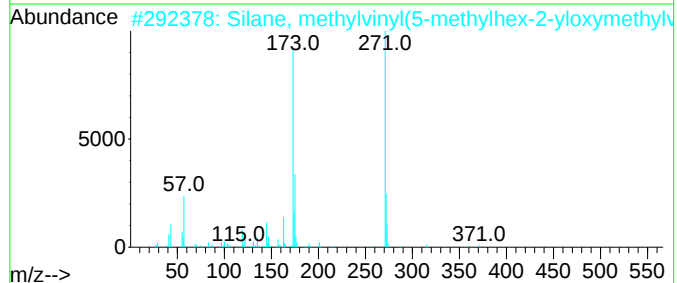
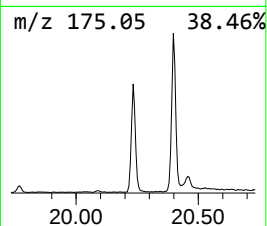
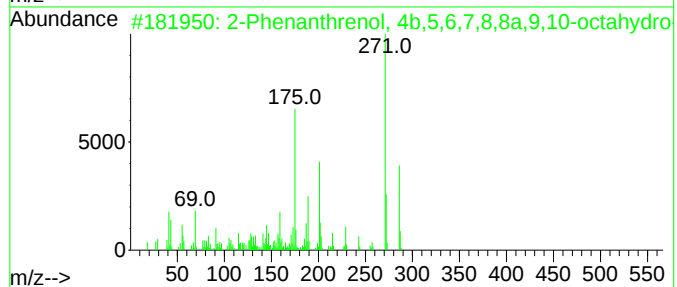
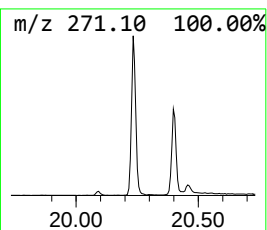
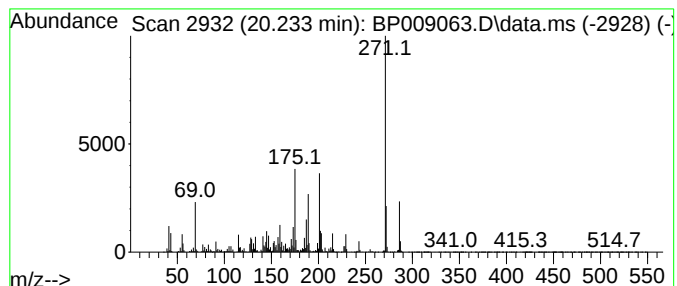
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown20.233 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.233	12.26 ng	1295720	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	93		
2	Silane, methylvinyl(5-methylhex-...	386	C20H42O3Si2	1000420-90-6	47		
3	Silane, methylvinyl(2-methylpent...	372	C19H40O3Si2	1010421-54-4	47		
4	Silane, methylvinyl(hept-2-yloxy...	386	C20H42O3Si2	1000415-93-0	47		
5	6-Bromo-2-chloroquinoline-3-carb...	269	C10H5BrClNO	073568-35-1	42		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020822\
Data File : BP009063.D
Acq On : 08 Feb 2022 17:45
Operator : CG/JU
Sample : N1421-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-4

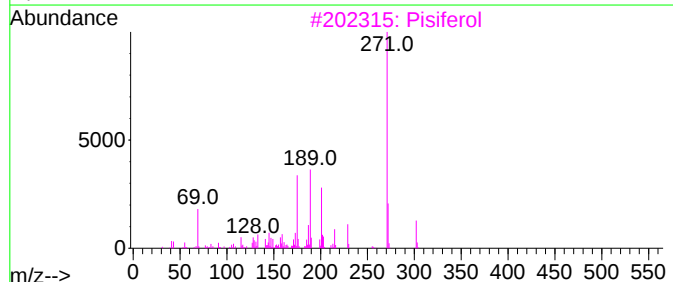
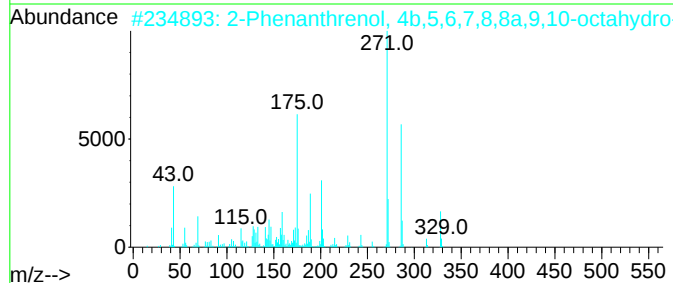
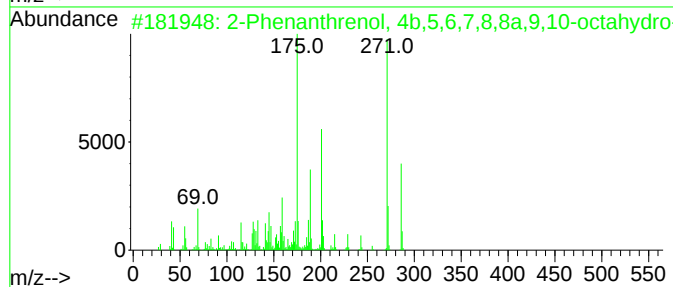
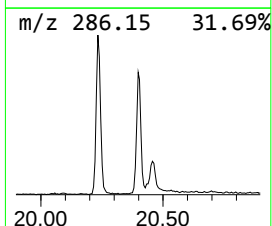
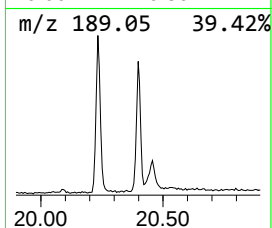
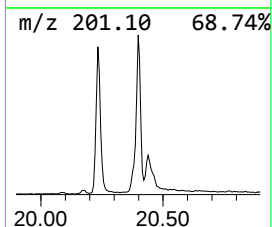
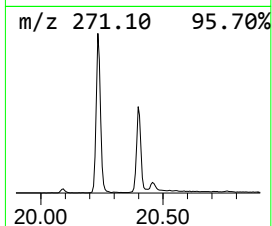
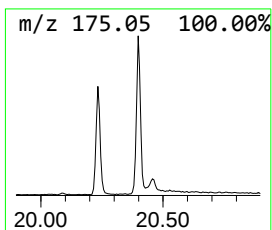
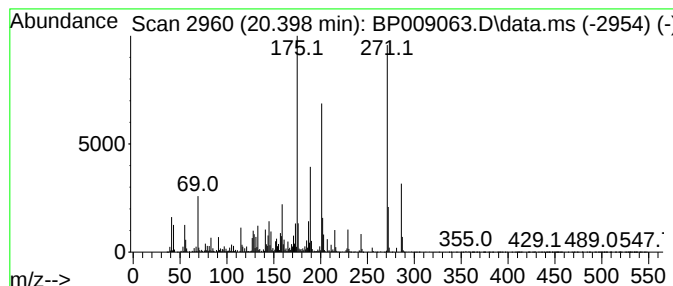
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown20.398 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.398	9.18 ng	970687	Chrysene-d12	21.298

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	90
3		Pisiferol	302	C20H30O2	024035-36-7	49
4		13-Isopropylpodocarpene-12-ol-20-al	300	C20H28O2	024035-37-8	47
5		(4Br,8As)-(+)-4B,5,6,7,8,8A,9,10...	346	C22H34O3	1000426-72-2	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020822\
Data File : BP009063.D
Acq On : 08 Feb 2022 17:45
Operator : CG/JU
Sample : N1421-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-4

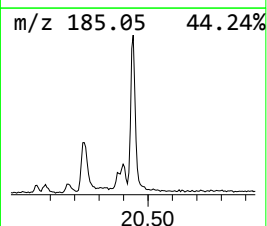
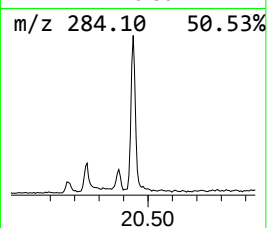
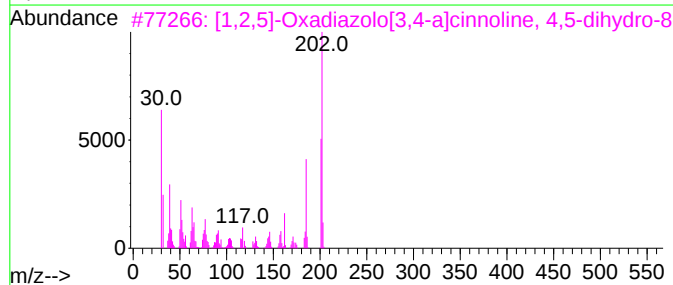
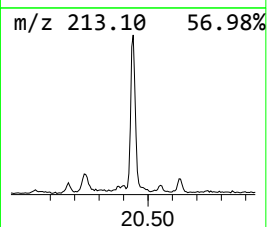
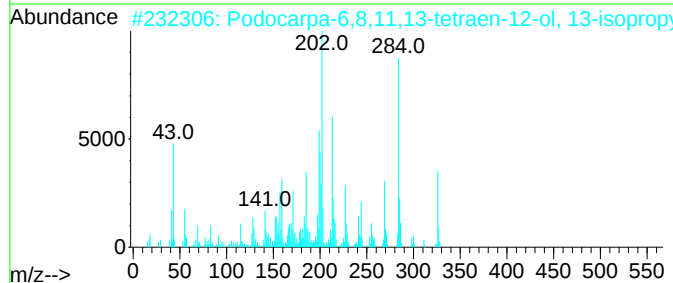
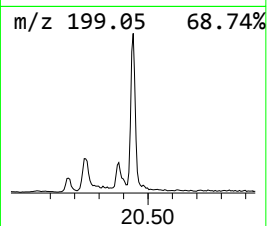
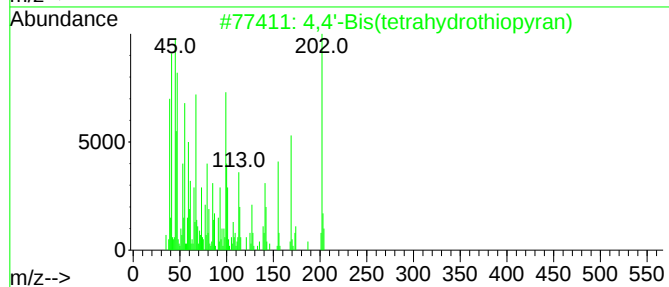
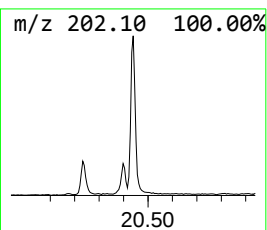
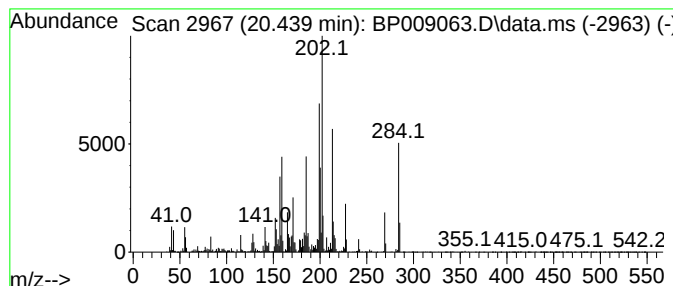
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.439	9.33 ng	986310	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	91
2			Podocarpa-6,8,11,13-tetraen-12-o...	326	C22H30O2	022160-86-7	43
3			[1,2,5]-Oxadiazolo[3,4-a]cinnoli...	202	C10H10N4O	1000260-59-4	20
4			5-Hydroxy-3-methyl-1-phenylpyraz...	202	C11H10N2O2	060484-29-9	18
5			Phosphorin, 2,6-bis(1,1-dimethyl...	284	C19H25P	017420-27-8	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020822\
Data File : BP009063.D
Acq On : 08 Feb 2022 17:45
Operator : CG/JU
Sample : N1421-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-4

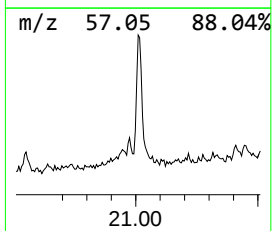
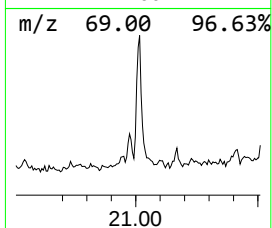
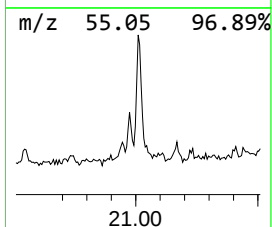
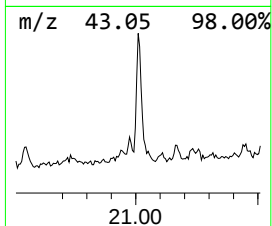
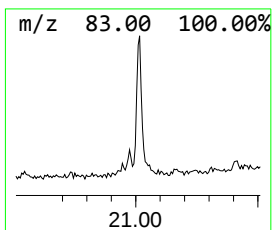
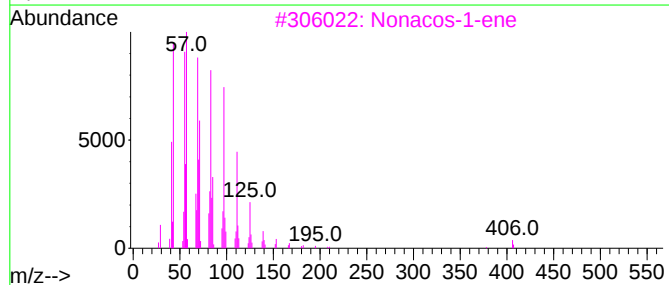
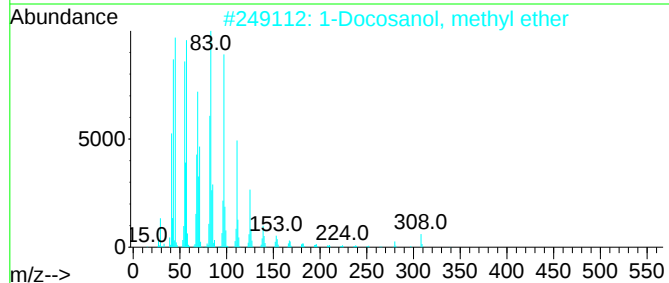
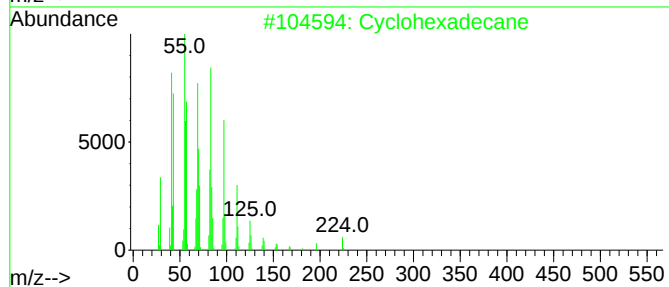
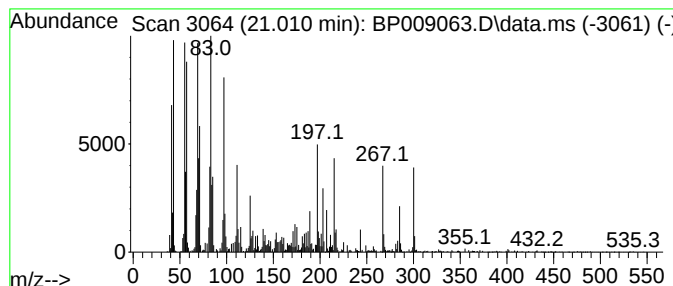
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclohexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	3.64 ng	385166	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	70
2			1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	64
3			Nonacos-1-ene	406	C29H58	018835-35-3	55
4			1-Tetracosene	336	C24H48	010192-32-2	55
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020822\
Data File : BP009063.D
Acq On : 08 Feb 2022 17:45
Operator : CG/JU
Sample : N1421-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-4

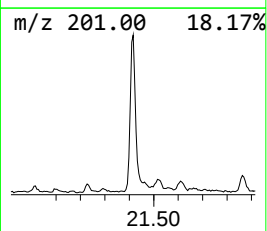
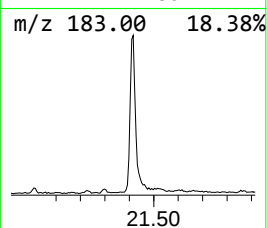
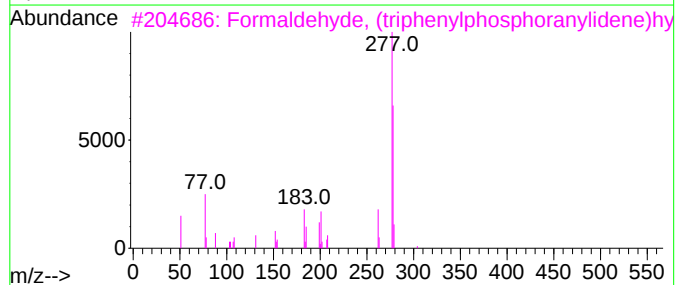
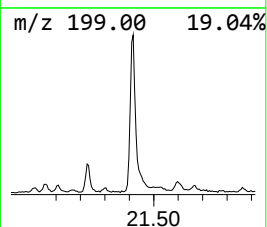
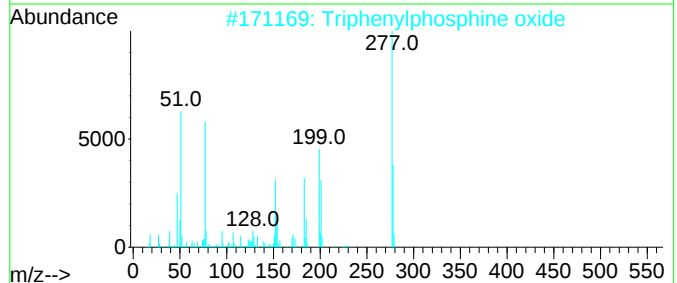
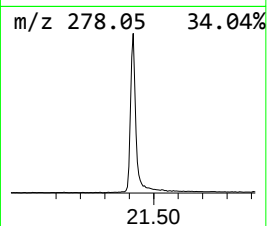
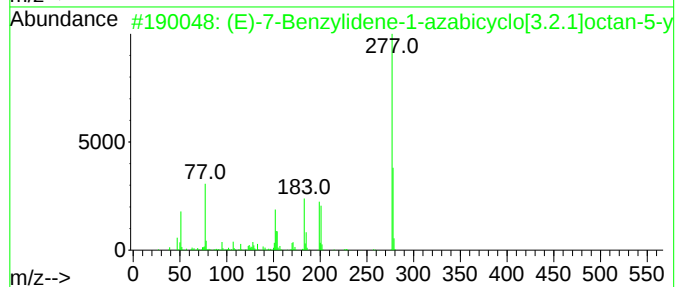
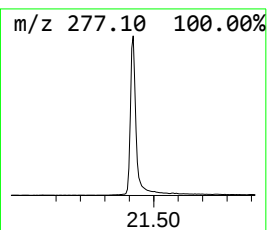
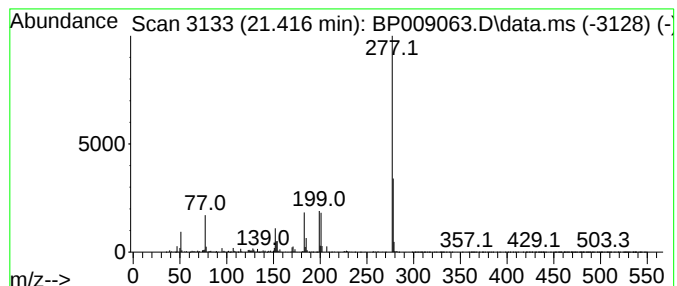
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 (E)-7-Benzylidene-1-azabicyclo... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	11.81 ng	1247940	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	86		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	83		
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38		
4	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28		
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020822\
Data File : BP009063.D
Acq On : 08 Feb 2022 17:45
Operator : CG/JU
Sample : N1421-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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...	3.017	5.4	ng	290239	1	7.804	1079980	20.0
Palmitoleic acid	18.045	4.9	ng	401525	4	17.204	1651440	20.0
n-Hexadecanoic ...	18.104	23.9	ng	1972010	4	17.204	1651440	20.0
Phenanthrene, 1...	19.027	13.6	ng	1126620	4	17.204	1651440	20.0
6-Octadecenoic ...	19.227	94.7	ng	7815210	4	17.204	1651440	20.0
Octadecanoic acid	19.339	8.6	ng	909053	5	21.298	2114220	20.0
unknown20.233	20.233	12.3	ng	1295720	5	21.298	2114220	20.0
unknown20.398	20.398	9.2	ng	970687	5	21.298	2114220	20.0
4,4'-Bis(tetra...	20.439	9.3	ng	986310	5	21.298	2114220	20.0
Cyclohexadecane	21.010	3.6	ng	385166	5	21.298	2114220	20.0
(E)-7-Benzylide...	21.416	11.8	ng	1247940	5	21.298	2114220	20.0