

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021122\
 Data File : BP009125.D
 Acq On : 11 Feb 2022 21:51
 Operator : CG/JU
 Sample : N1495-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 NB-08-021022

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: BP009125.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.387	402	408	435	rBV	2451064	4314431	28.81%	3.732%
2	6.987	673	680	696	rBV	2676379	4761204	31.79%	4.119%
3	7.793	807	817	825	rBV	651363	1128617	7.54%	0.976%
4	8.957	1007	1015	1024	rBV	1618119	3027432	20.22%	2.619%
5	10.587	1281	1292	1308	rBV	1000604	1890265	12.62%	1.635%
6	13.057	1704	1712	1725	rBV	5642972	8760795	58.50%	7.579%
7	14.157	1894	1899	1906	rVB	131409	201328	1.34%	0.174%
8	14.434	1939	1946	1953	rVV	1888599	2905424	19.40%	2.513%
9	14.498	1953	1957	1966	rVB	175534	273504	1.83%	0.237%
10	14.839	2010	2015	2020	rBV	109610	157711	1.05%	0.136%
11	15.486	2120	2125	2138	rVB	227117	387588	2.59%	0.335%
12	15.933	2194	2201	2221	rBV	5127821	8135617	54.33%	7.038%
13	16.163	2235	2240	2248	rVB6	81916	191388	1.28%	0.166%
14	17.010	2380	2384	2393	rVB2	166328	275005	1.84%	0.238%
15	17.192	2409	2415	2419	rBV	2554564	3833144	25.60%	3.316%
16	17.233	2419	2422	2429	rVV	2012576	2797614	18.68%	2.420%
17	17.328	2433	2438	2444	rVB	681330	995124	6.65%	0.861%
18	17.610	2482	2486	2493	rVB	114073	175982	1.18%	0.152%
19	17.869	2526	2530	2534	rVB	228409	273234	1.82%	0.236%
20	18.063	2559	2563	2565	rBV	270997	356231	2.38%	0.308%
21	18.092	2565	2568	2580	rVV2	737179	1575962	10.52%	1.363%
22	18.192	2581	2585	2590	rVV	197135	304387	2.03%	0.263%
23	18.251	2590	2595	2599	rVV3	537454	960962	6.42%	0.831%
24	18.286	2599	2601	2606	rVB	208290	265620	1.77%	0.230%
25	18.545	2642	2645	2650	rVV	196587	256406	1.71%	0.222%
26	18.969	2710	2717	2720	rBV2	471945	866332	5.79%	0.749%
27	19.004	2720	2723	2728	rVB3	409619	581744	3.88%	0.503%
28	19.210	2752	2758	2765	rBV	5723050	8112372	54.17%	7.018%
29	19.327	2772	2778	2781	rBV2	257656	487636	3.26%	0.422%
30	19.533	2809	2813	2814	rBV	969500	1124644	7.51%	0.973%
31	19.563	2814	2818	2826	rVB	4880402	7370582	49.22%	6.376%
32	19.633	2826	2830	2836	rBV2	248615	352977	2.36%	0.305%
33	19.757	2845	2851	2856	rBV	10817396	14975463	100.00%	12.955%
34	19.886	2867	2873	2879	rBV2	293289	721672	4.82%	0.624%
35	20.051	2890	2901	2906	rBV	901915	2033088	13.58%	1.759%
36	20.145	2913	2917	2921	rBV	700199	907154	6.06%	0.785%

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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

37	20.198	2924	2926	2930	rVB	370107	476837	3.18%	0.413%
38	20.339	2947	2950	2953	rBV	247531	304652	2.03%	0.264%
39	20.380	2955	2957	2961	rVB	225230	283199	1.89%	0.245%
40	20.939	3050	3052	3055	rBV	324211	416130	2.78%	0.360%
41	20.998	3056	3062	3064	rBV2	1513502	2549586	17.03%	2.206%
42	21.286	3105	3111	3115	rBV2	3799237	7907660	52.80%	6.841%
43	21.327	3115	3118	3122	rVB	2134316	2613680	17.45%	2.261%
44	21.404	3127	3131	3136	rBV2	2588343	4387818	29.30%	3.796%
45	22.957	3389	3395	3400	rBV2	1388749	3548160	23.69%	3.069%
46	23.580	3495	3501	3508	rBV	1274726	3258496	21.76%	2.819%
47	23.686	3514	3519	3525	rVB3	1911752	4111879	27.46%	3.557%

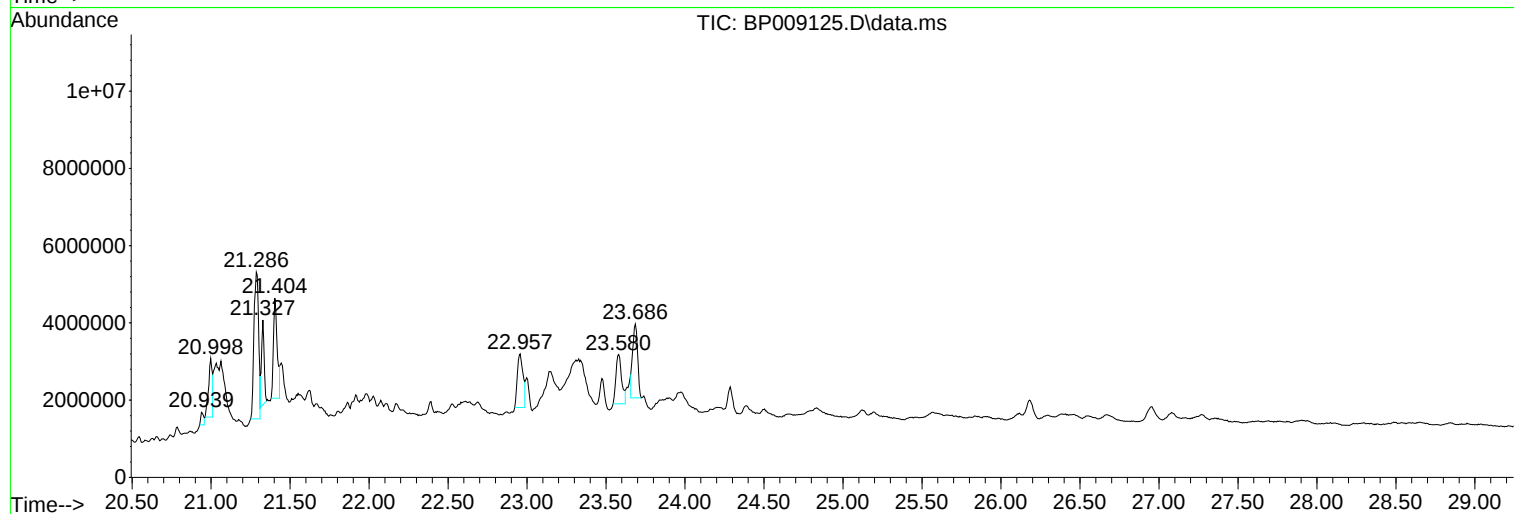
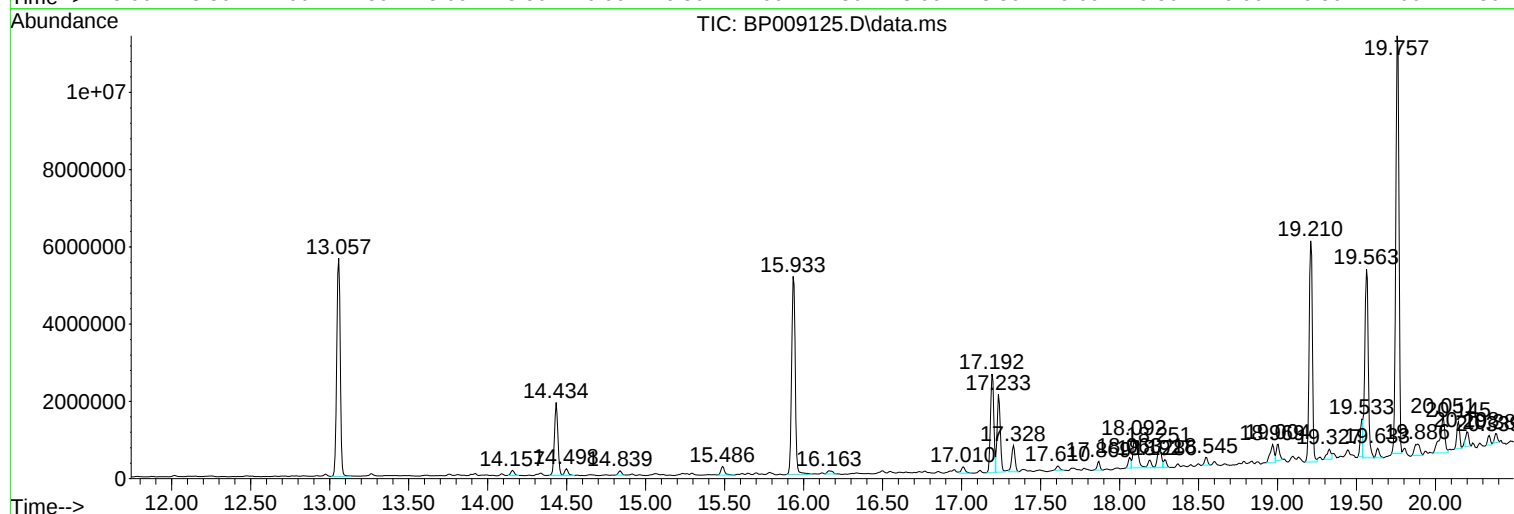
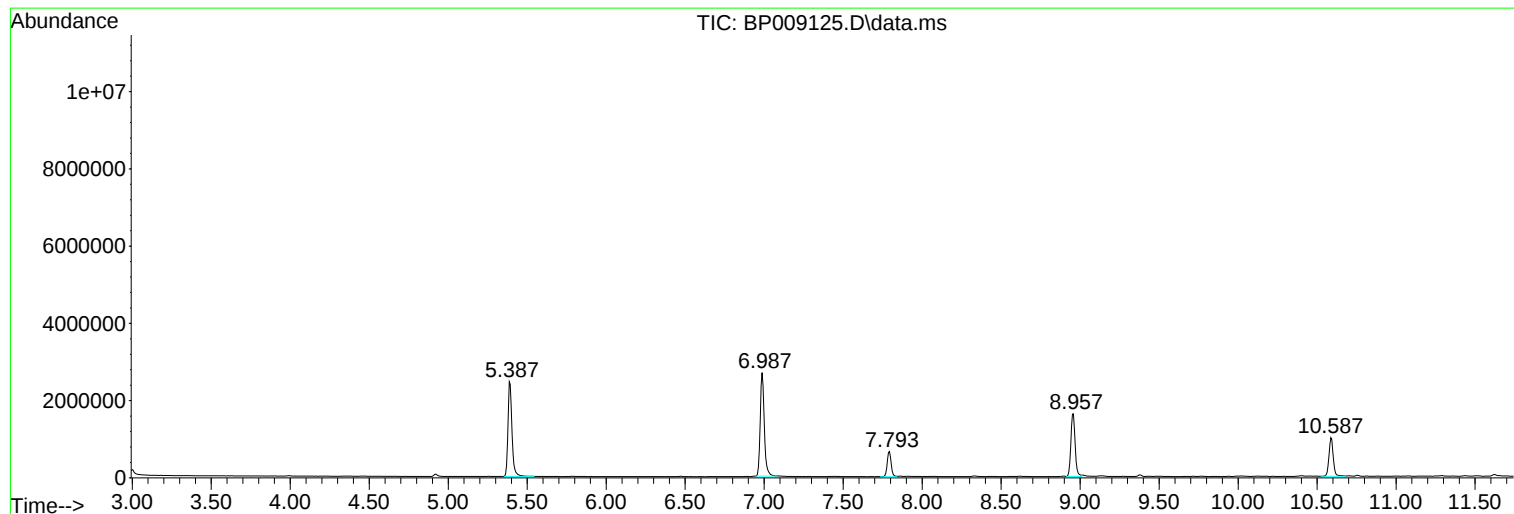
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Acq On : 11 Feb 2022 21:51
Operator : CG/JU
Sample : N1495-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

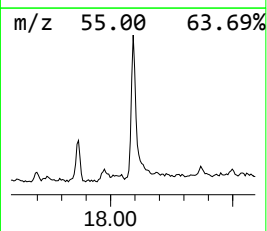
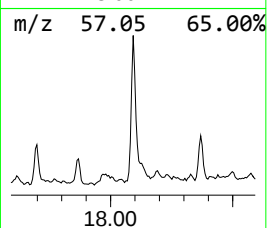
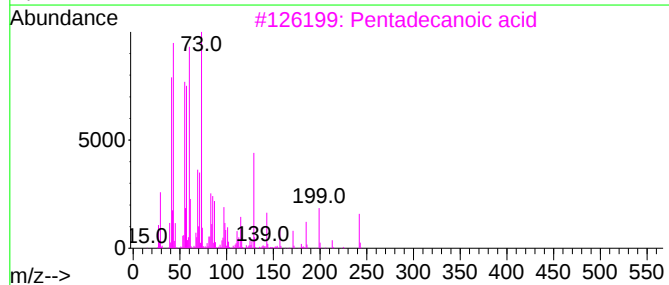
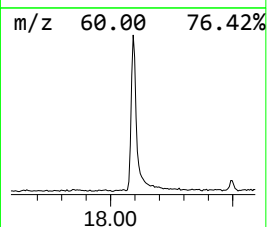
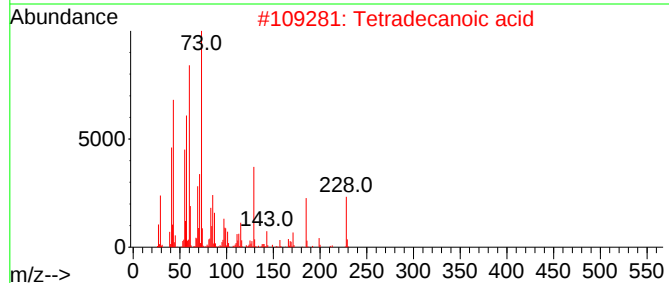
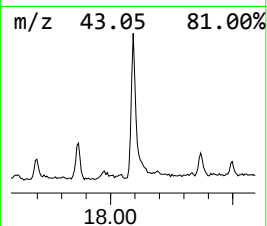
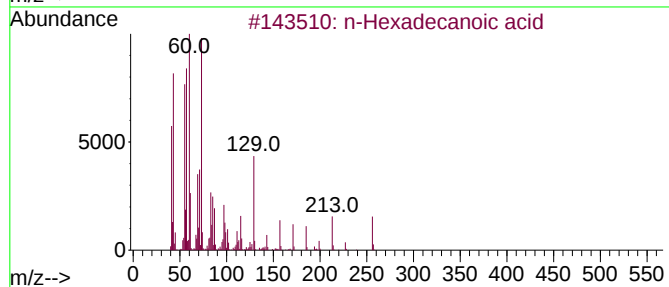
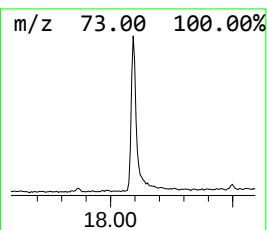
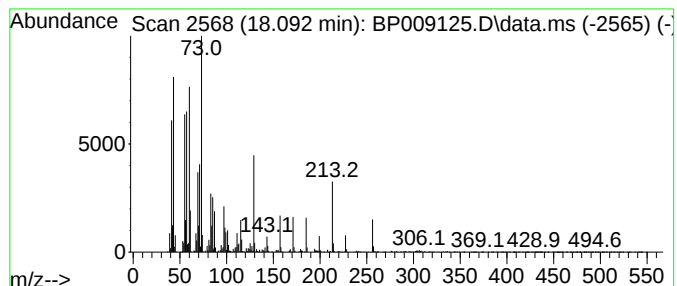
Instrument :
BNA_P
ClientSampleId :
NB-08-021022

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.092	8.22 ng	1575960	Phenanthrene-d10	17.192	
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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76



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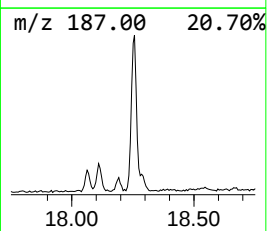
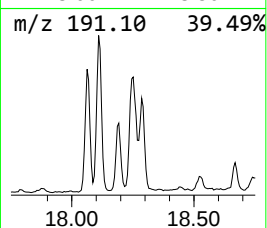
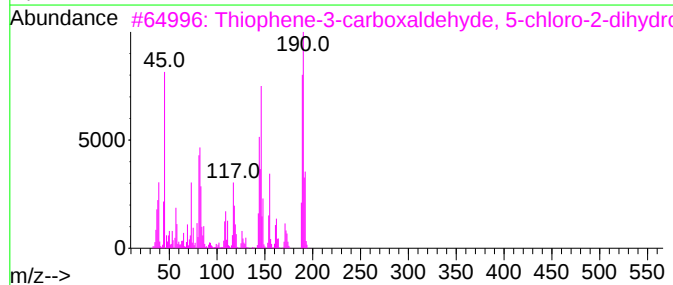
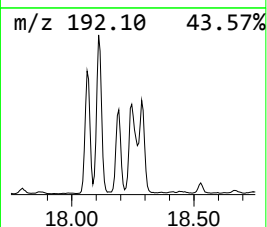
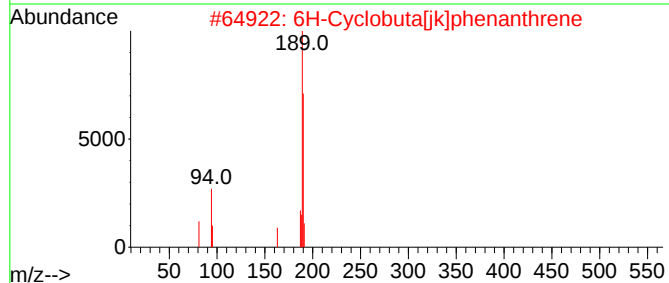
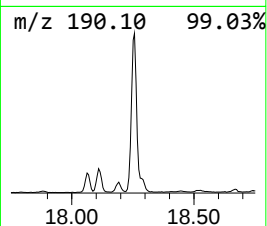
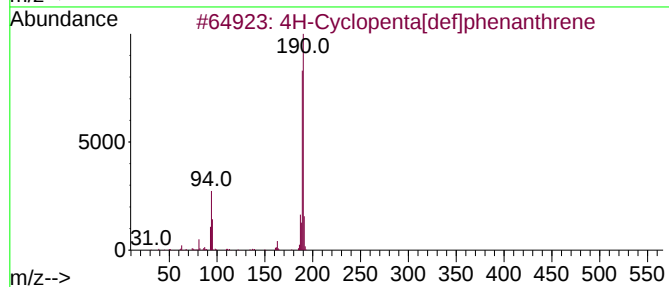
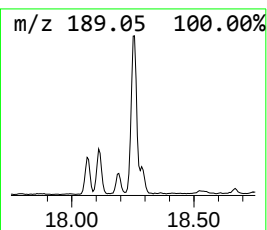
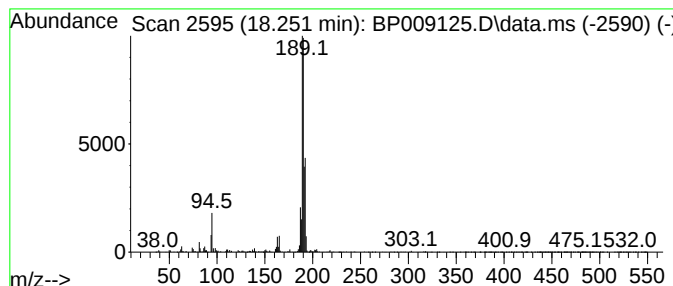
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BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.251	5.01 ng	960962	Phenanthrene-d10	17.192	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
5	Methyl diselenide	190	C2H6Se2	007101-31-7	45



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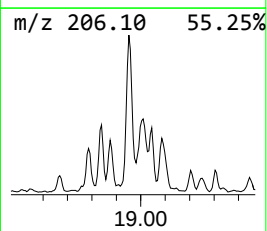
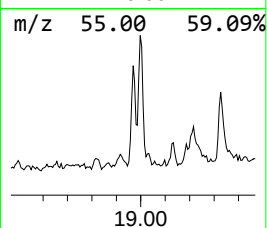
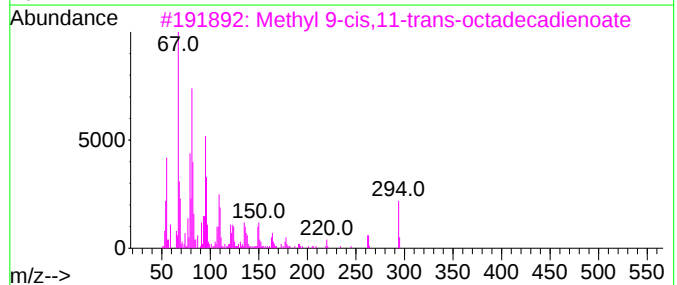
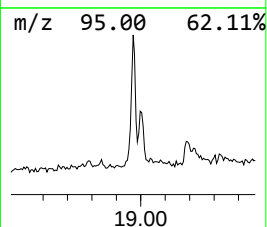
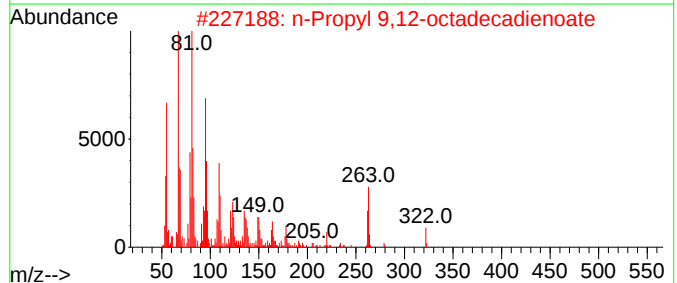
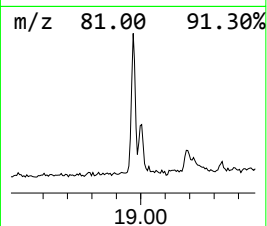
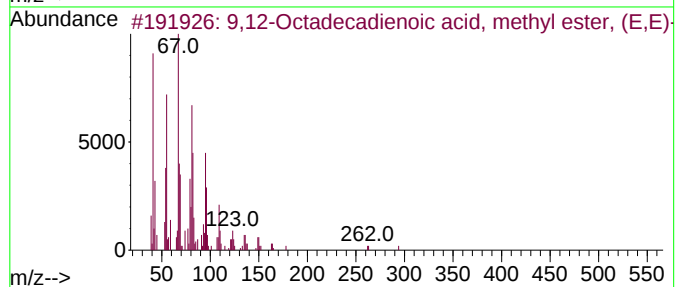
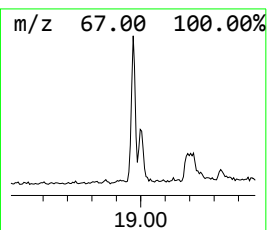
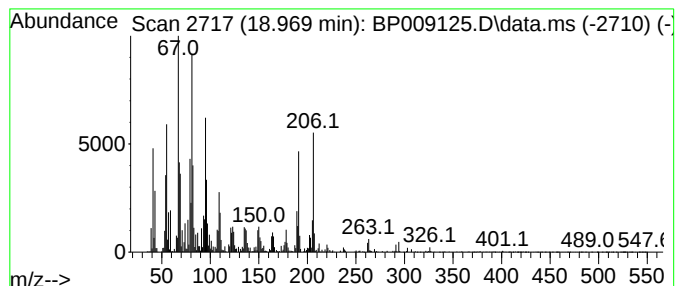
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.969	4.52 ng	866332	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	97
2			n-Propyl 9,12-octadecadienoate	322	C21H38O2	1000336-77-8	95
3			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	95
4			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
5			Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	95



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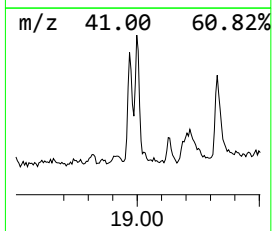
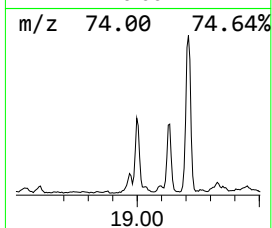
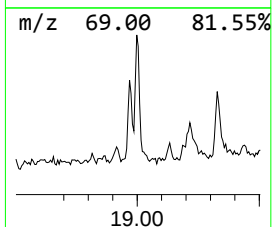
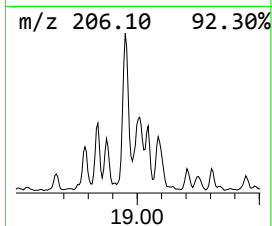
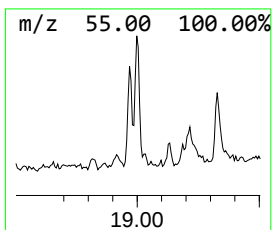
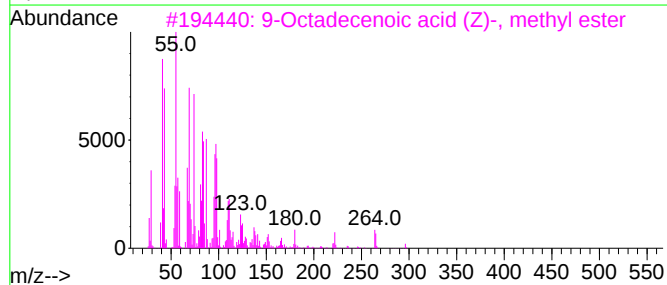
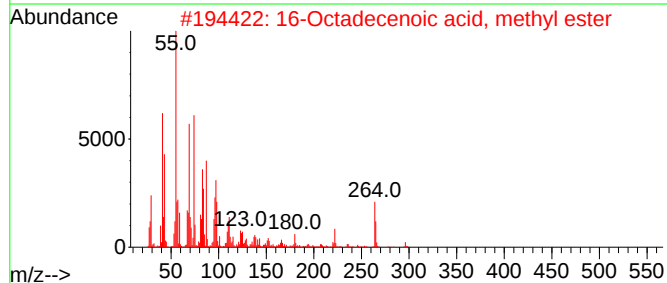
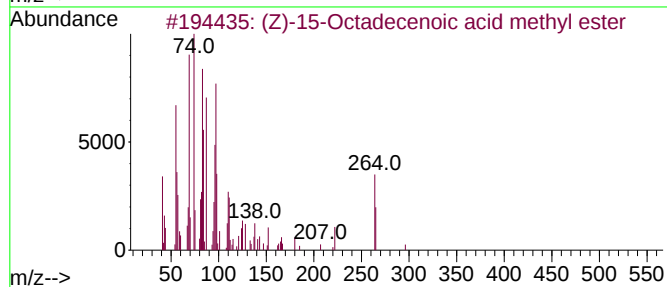
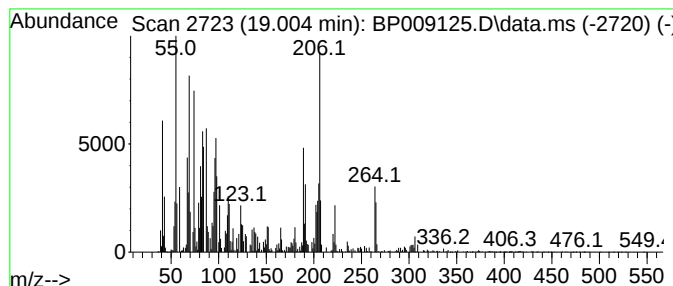
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (Z)-15-Octadecenoic acid me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.004	3.04 ng	581744	Phenanthrene-d10	17.192	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	99
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	98
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	95
5	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	95



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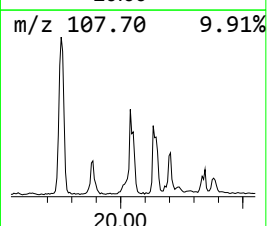
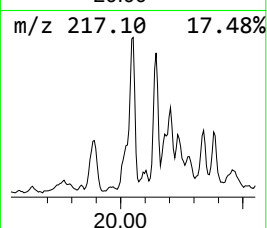
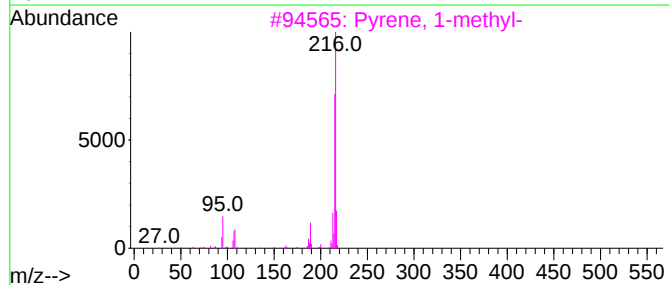
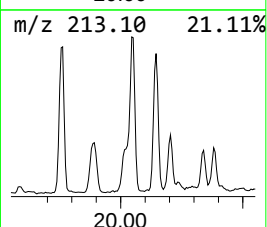
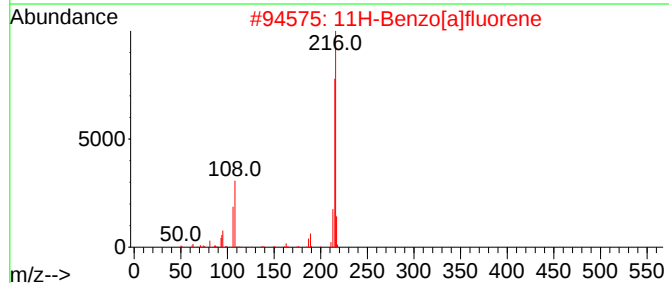
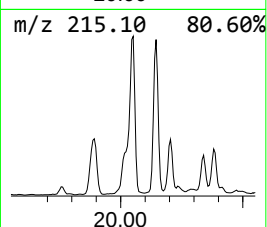
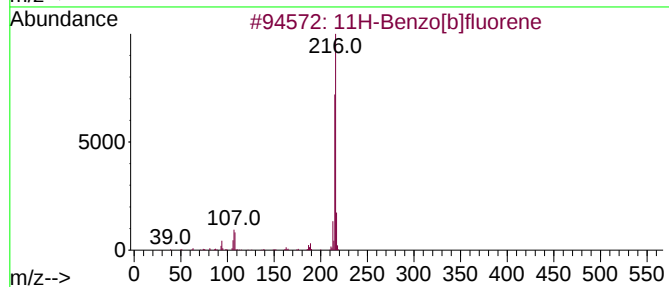
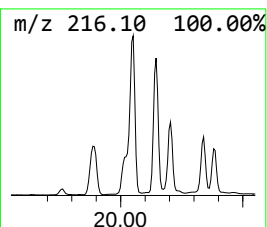
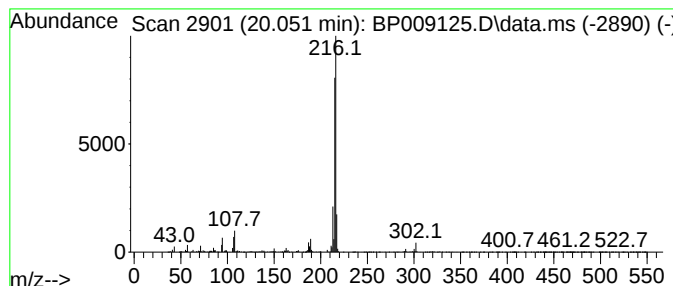
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 11H-Benzo[b]fluorene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.051	5.14 ng	2033090	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
3			Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
5			Pyrene, 2-methyl-	216	C17H12	003442-78-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021122\
Data File : BP009125.D
Acq On : 11 Feb 2022 21:51
Operator : CG/JU
Sample : N1495-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-08-021022

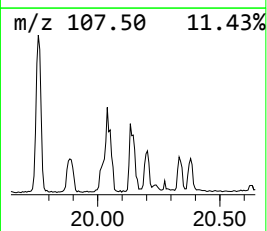
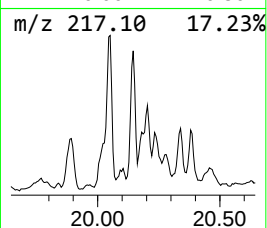
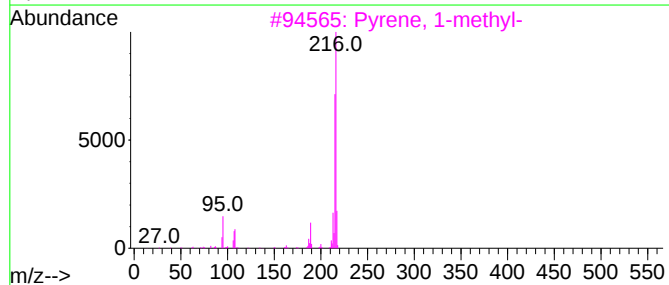
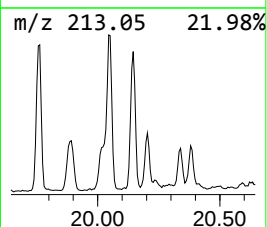
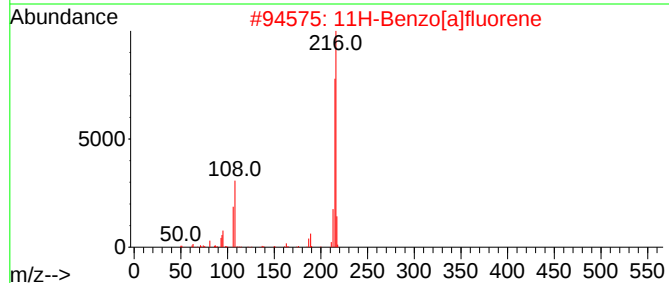
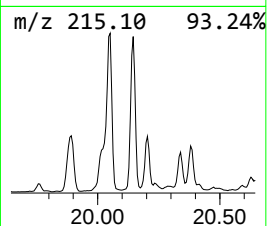
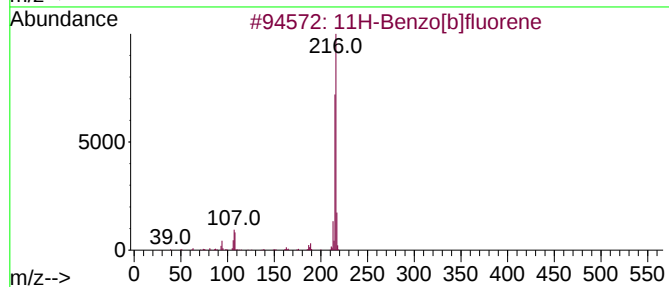
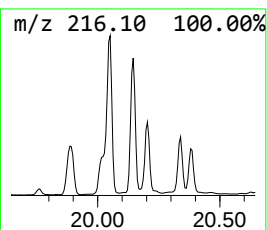
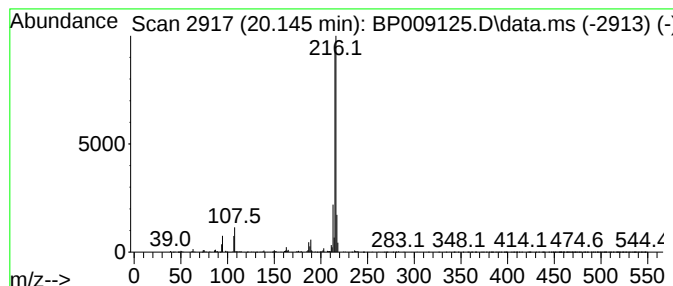
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 11H-Benzo[a]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.145	2.29 ng	907154	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3			Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
4			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87
5			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021122\
Data File : BP009125.D
Acq On : 11 Feb 2022 21:51
Operator : CG/JU
Sample : N1495-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-08-021022

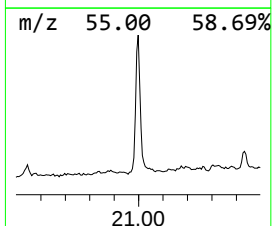
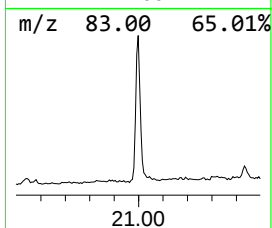
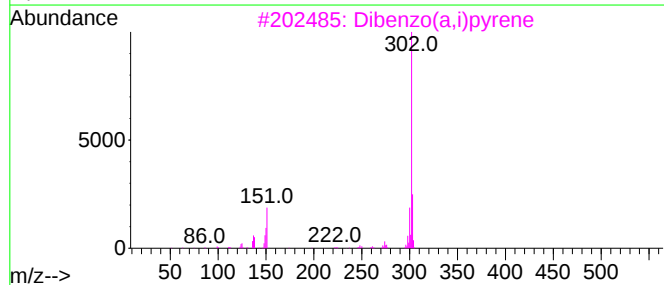
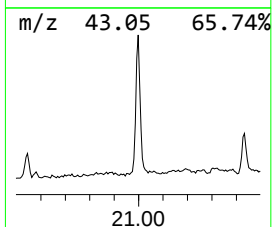
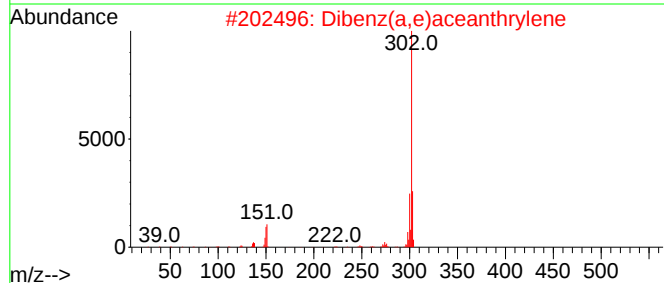
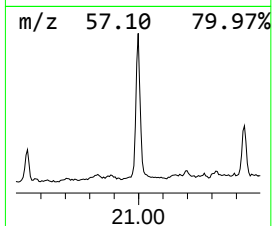
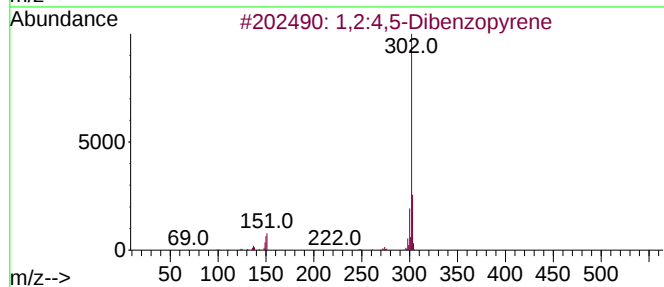
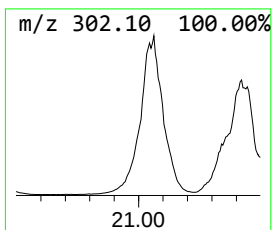
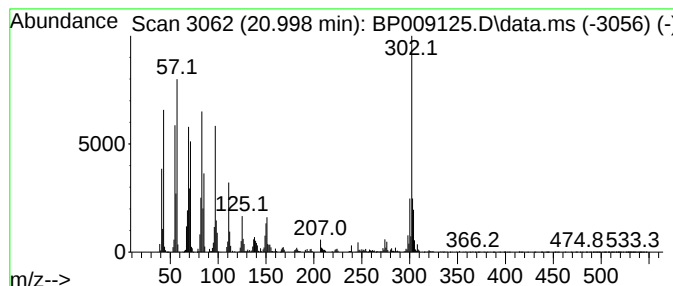
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,2:4,5-Dibenzopyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.998	6.45 ng	2549590	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	97
2			Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	96
3			Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	95
4			3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	91
5			Dibenzo[fg,op]naphthacene	302	C24H14	000192-51-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021122\
Data File : BP009125.D
Acq On : 11 Feb 2022 21:51
Operator : CG/JU
Sample : N1495-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-08-021022

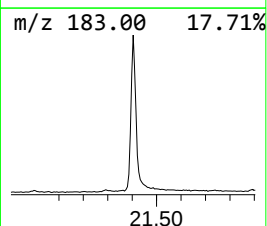
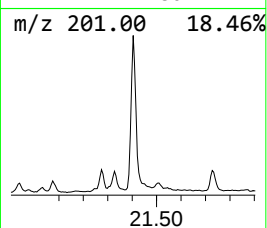
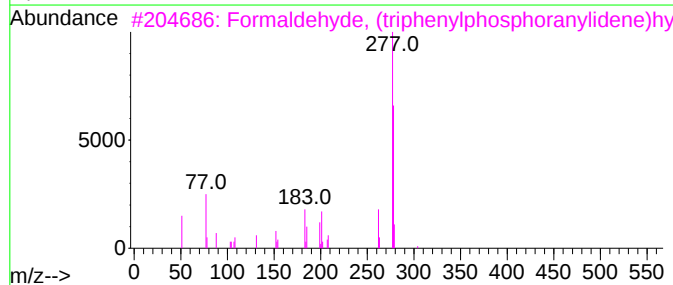
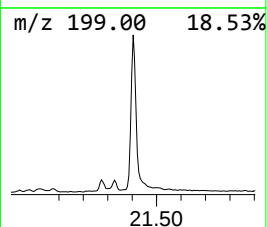
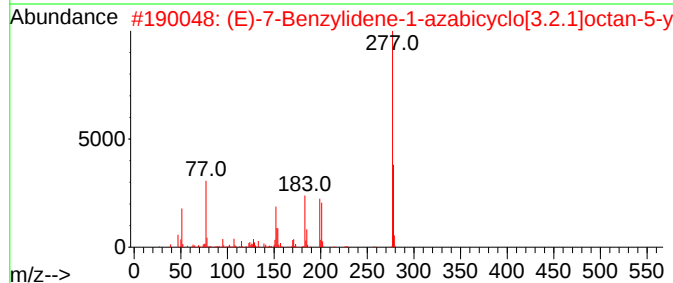
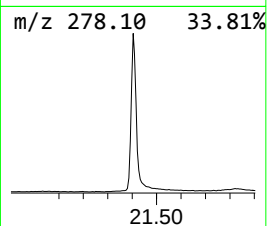
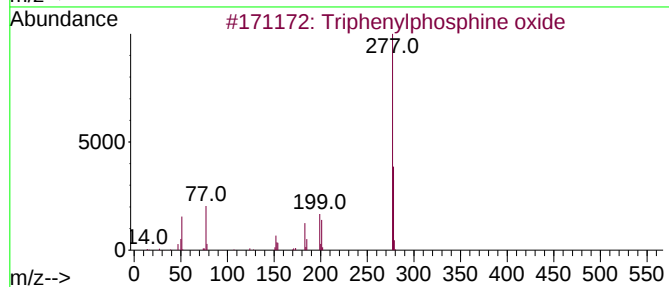
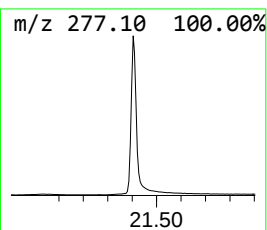
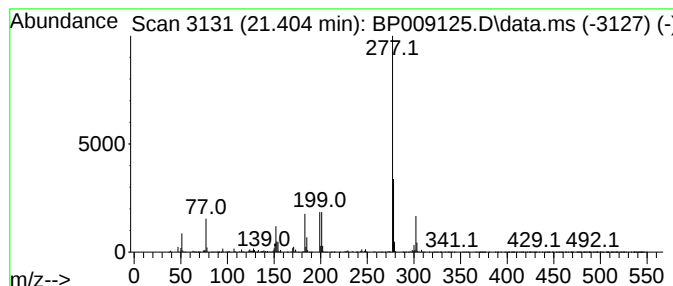
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.404	11.10 ng	4387820	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	86
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	46
4			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	37
5			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021122\
Data File : BP009125.D
Acq On : 11 Feb 2022 21:51
Operator : CG/JU
Sample : N1495-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-08-021022

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
n-Hexadecanoic ...	18.092	8.2	ng	1575960	4	17.192	3833140	20.0
4H-Cyclopenta[d]...	18.251	5.0	ng	960962	4	17.192	3833140	20.0
9,12-Octadecadi...	18.969	4.5	ng	866332	4	17.192	3833140	20.0
(Z)-15-Octadece...	19.004	3.0	ng	581744	4	17.192	3833140	20.0
11H-Benzo[b]flu...	20.051	5.1	ng	2033090	5	21.292	7907660	20.0
11H-Benzo[a]flu...	20.145	2.3	ng	907154	5	21.292	7907660	20.0
1,2:4,5-Dibenzo...	20.998	6.5	ng	2549590	5	21.292	7907660	20.0
Triphenylphosph...	21.404	11.1	ng	4387820	5	21.292	7907660	20.0