

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
 Data File : BP016459.D
 Acq On : 01 Aug 2023 16:46
 Operator : MA/JU
 Sample : 03715-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 T842-FH-02-CT

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-BP072723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP016459.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.140	311	315	322	rVB	268819	382526	1.19%	0.196%
2	5.587	384	391	400	rBV	7272871	11066819	34.46%	5.667%
3	7.216	660	668	684	rBV	7453237	12106221	37.70%	6.200%
4	8.075	807	814	824	rBV	2021910	3266970	10.17%	1.673%
5	9.275	1008	1018	1030	rBV	4677435	7667532	23.88%	3.927%
6	10.910	1288	1296	1304	rBV	2866446	4820905	15.01%	2.469%
7	13.351	1698	1711	1720	rBV	11786001	17487478	54.46%	8.956%
8	14.340	1874	1879	1894	rBV	517497	770188	2.40%	0.394%
9	14.728	1936	1945	1954	rVB	4138950	6093484	18.97%	3.121%
10	16.104	2171	2179	2185	rBV	20822623	32113509	100.00%	16.446%
11	16.228	2191	2200	2215	rBV	8030515	12466052	38.82%	6.384%
12	16.698	2275	2280	2289	rVB	274047	392676	1.22%	0.201%
13	16.845	2299	2305	2317	rBV2	222487	356099	1.11%	0.182%
14	17.492	2407	2415	2426	rVB	4984887	7209931	22.45%	3.692%
15	18.216	2534	2538	2546	rVB2	261986	391496	1.22%	0.200%
16	18.345	2553	2560	2571	rBV	5224727	7443731	23.18%	3.812%
17	18.739	2623	2627	2632	rVB	328716	383701	1.19%	0.196%
18	19.163	2695	2699	2705	rBV	266995	383271	1.19%	0.196%
19	19.457	2740	2749	2761	rBV	634173	1495352	4.66%	0.766%
20	19.575	2764	2769	2792	rVB	2930320	4461486	13.89%	2.285%
21	19.857	2813	2817	2820	rBV	460652	548251	1.71%	0.281%
22	19.898	2820	2824	2838	rVB	1511151	2048639	6.38%	1.049%
23	20.039	2842	2848	2853	rBV	18025995	22843398	71.13%	11.698%
24	20.710	2958	2962	2966	rVB	718612	847102	2.64%	0.434%
25	20.786	2972	2975	2986	rVB4	238044	462187	1.44%	0.237%
26	21.122	3029	3032	3038	rBV4	293078	378946	1.18%	0.194%
27	21.251	3049	3054	3064	rBV	1805291	2498354	7.78%	1.279%
28	21.457	3086	3089	3093	rVB	334668	362454	1.13%	0.186%
29	21.586	3106	3111	3120	rVB	4624220	6288250	19.58%	3.220%
30	22.192	3210	3214	3218	rBV	254485	362600	1.13%	0.186%
31	22.498	3262	3266	3275	rVB	510876	749715	2.33%	0.384%
32	22.727	3302	3305	3317	rVB2	203041	458480	1.43%	0.235%
33	22.880	3326	3331	3343	rVB	2578679	3871368	12.06%	1.983%
34	24.186	3546	3553	3568	rVB	2510613	5565917	17.33%	2.850%
35	24.698	3631	3640	3656	rVB	4710469	11044798	34.39%	5.656%
36	25.727	3807	3815	3837	rBV2	2061116	6178604	19.24%	3.164%

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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-BP072723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

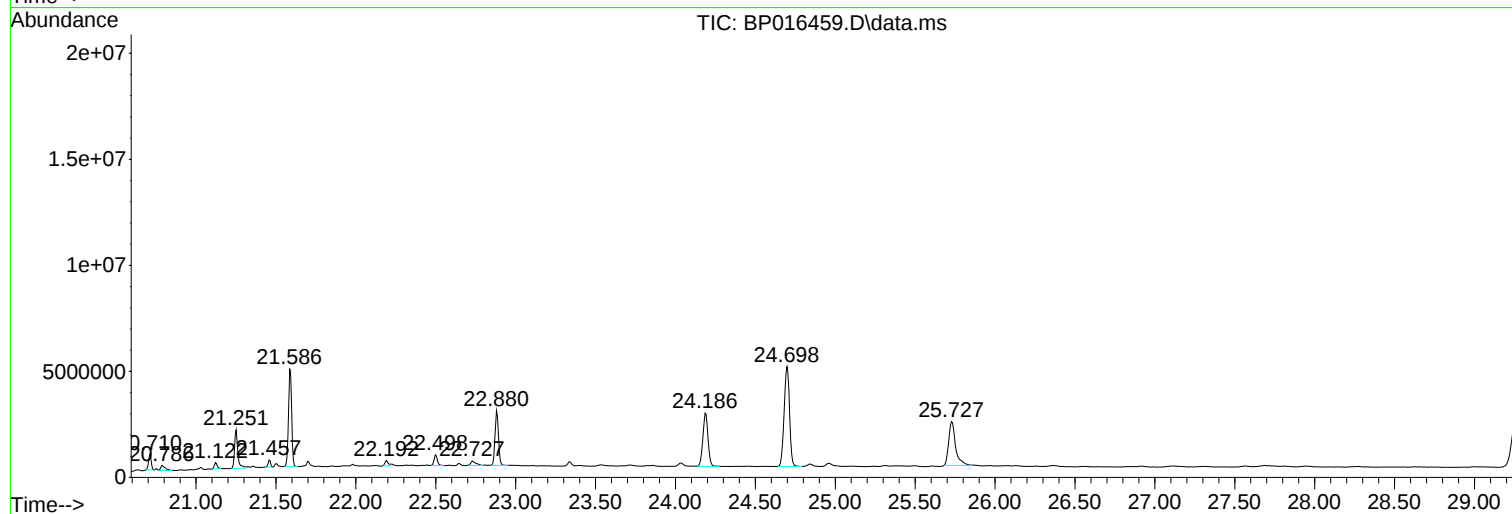
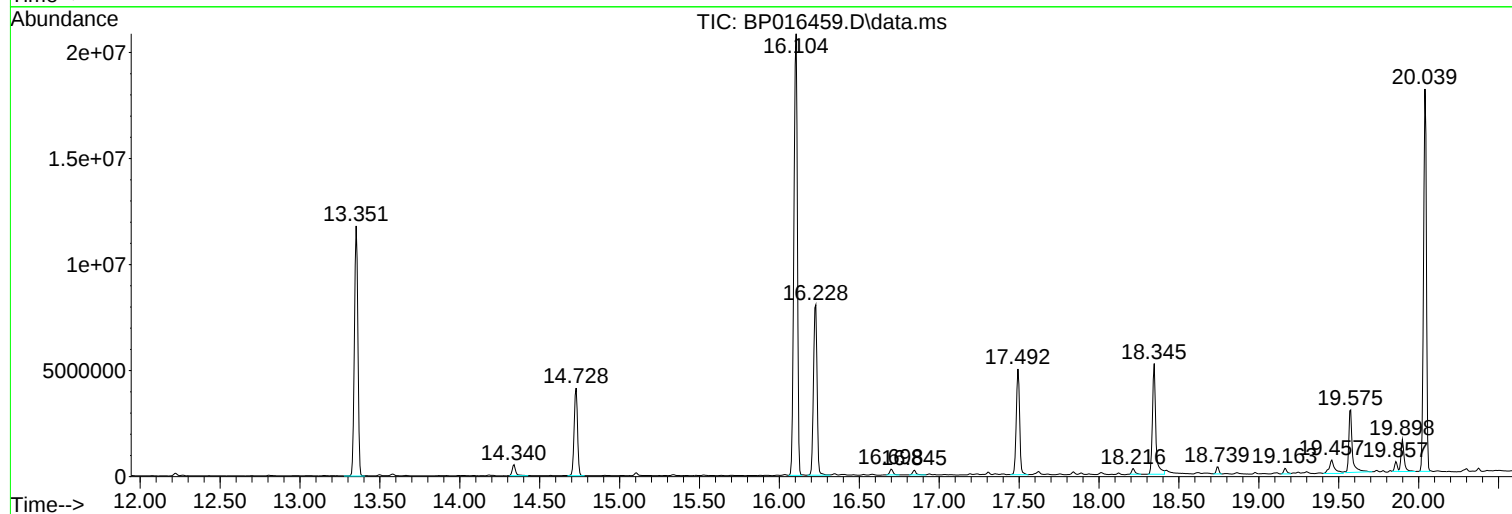
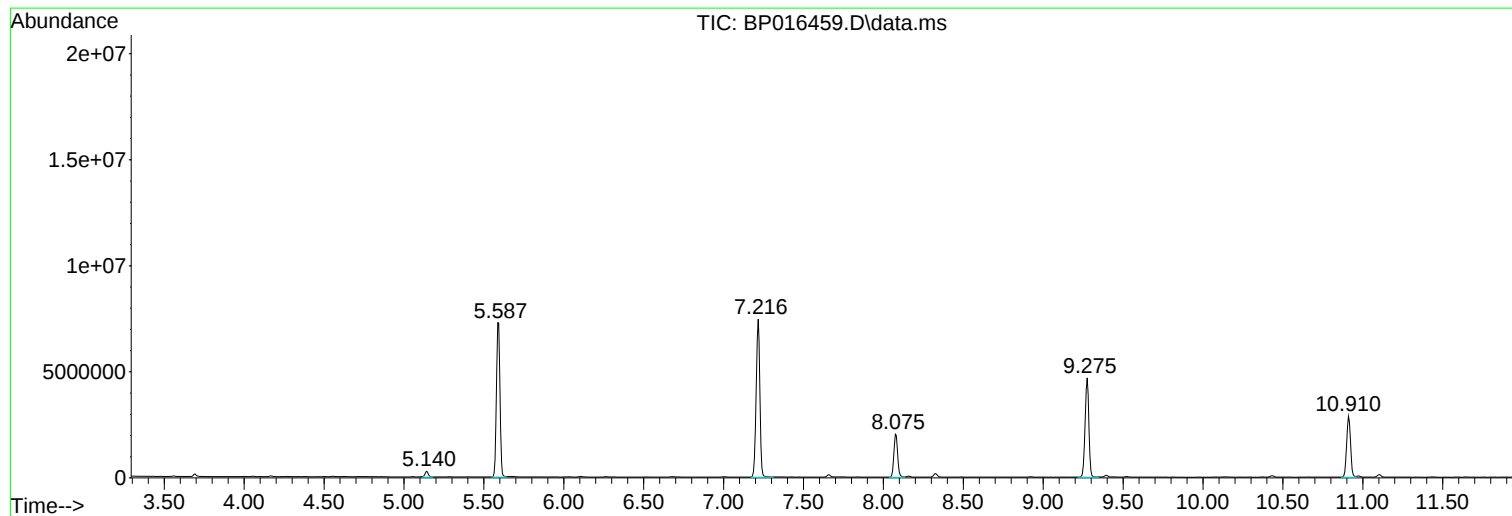
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ClientSampleId :
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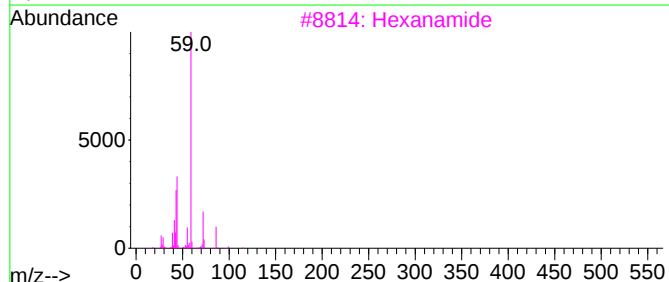
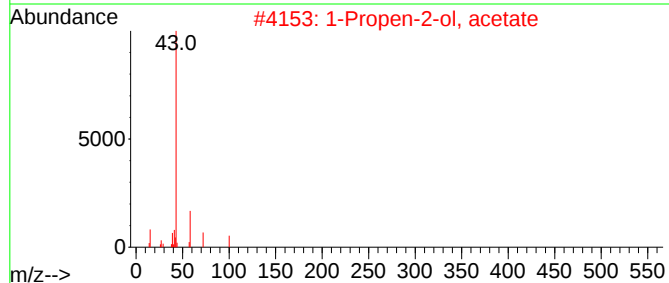
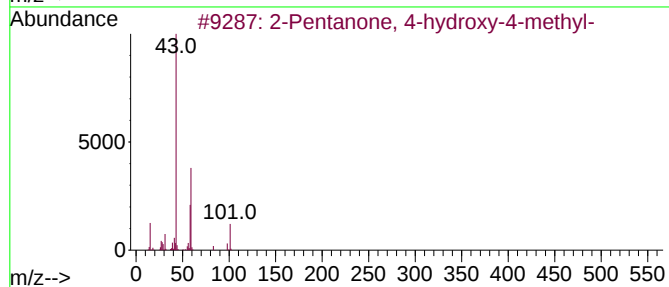
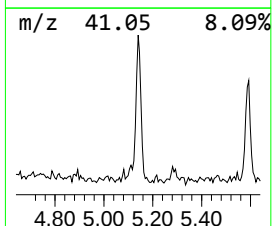
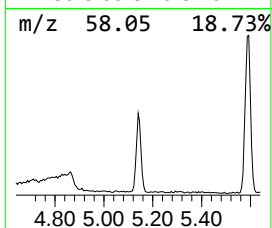
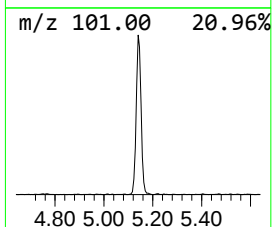
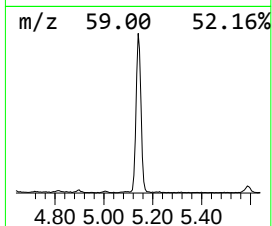
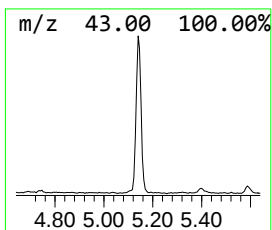
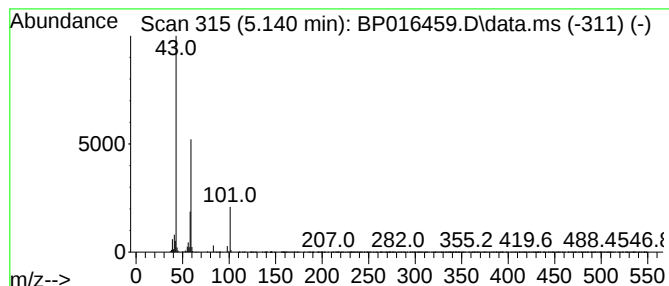
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	2.34 ng	382526	1,4-Dichlorobenzene-d4	8.075

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			Hexanamide	115	C6H13NO	000628-02-4	9
4			Acetone	58	C3H6O	000067-64-1	9
5			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9



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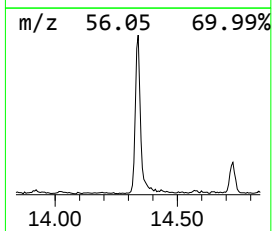
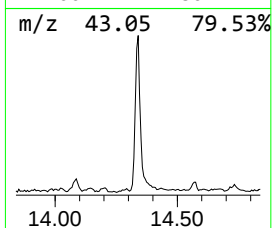
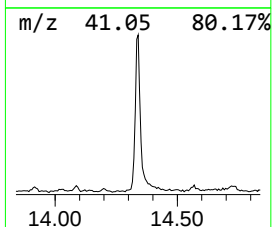
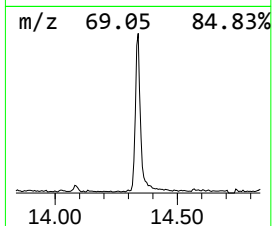
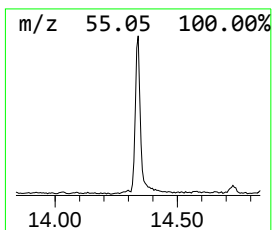
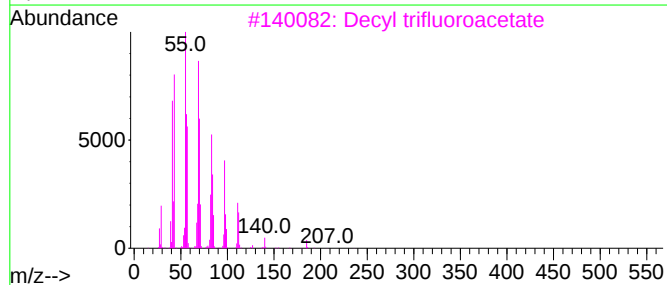
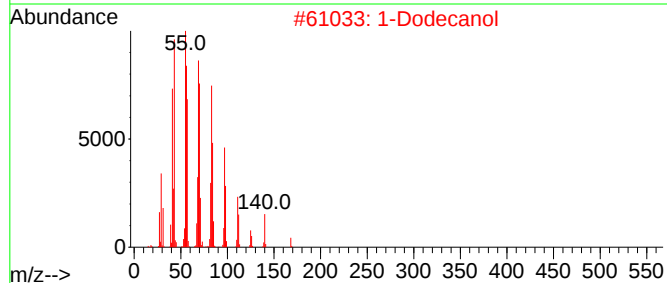
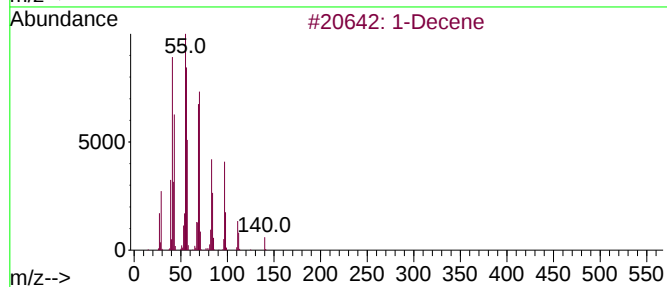
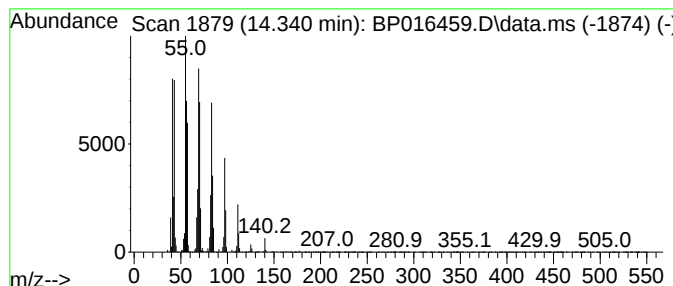
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Peak Number 2 1-Decene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.339	2.53 ng	770188	Acenaphthene-d10	14.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decene	140	C10H20	000872-05-9	93
2			1-Dodecanol	186	C12H26O	000112-53-8	91
3			Decyl trifluoroacetate	254	C12H21F3O2	000333-88-0	91
4			Pentadecafluorooctanoic acid, un...	568	C19H23F15O2	1010406-04-1	91
5			Carbonochloridic acid, decyl ester	220	C11H21ClO2	055488-51-2	91



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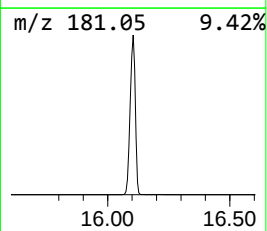
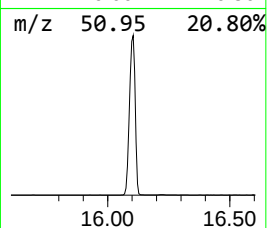
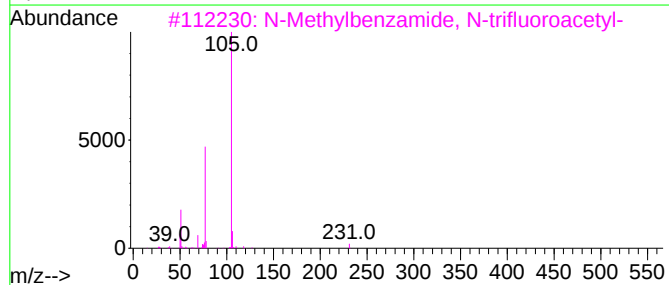
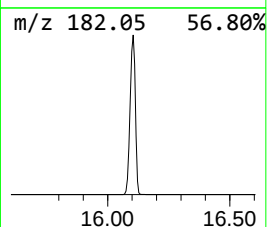
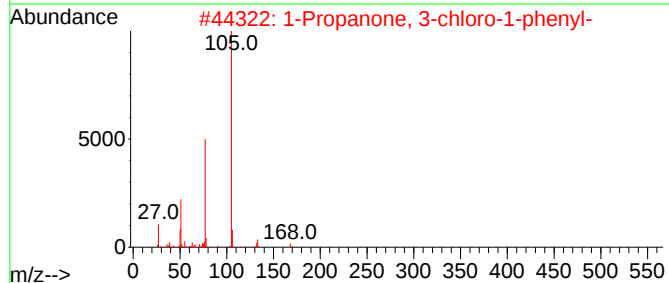
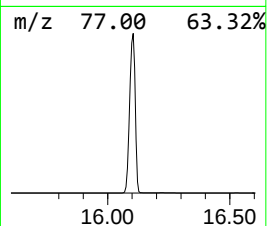
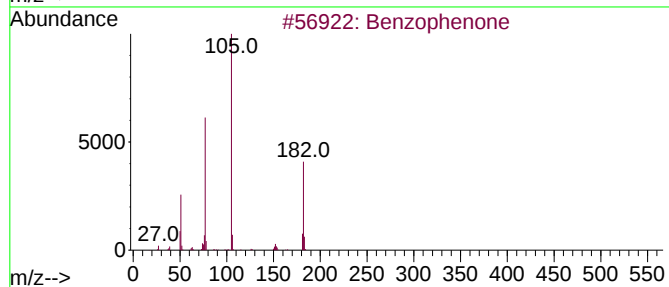
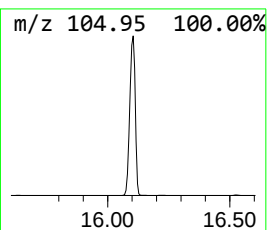
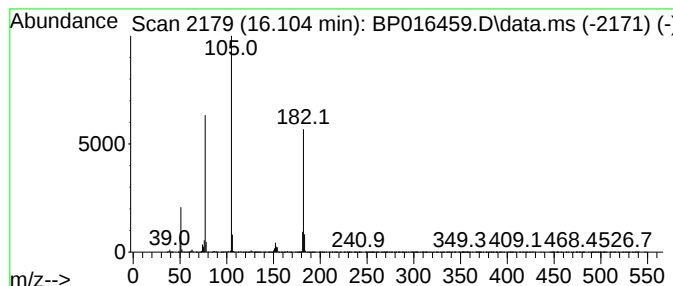
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	105.40 ng	32113500	Acenaphthene-d10	14.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
3			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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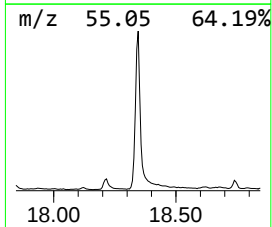
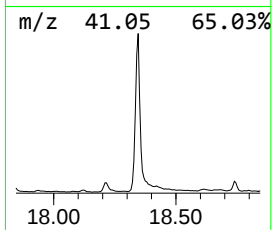
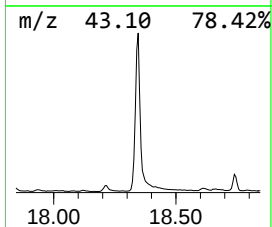
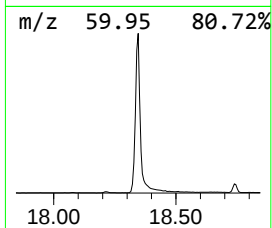
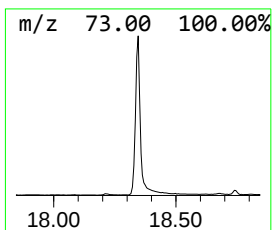
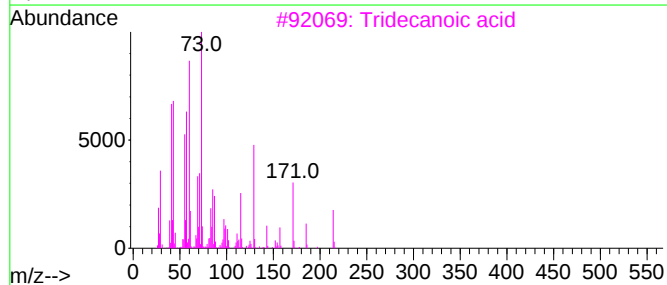
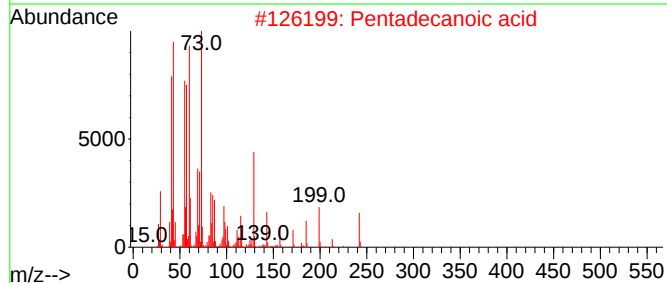
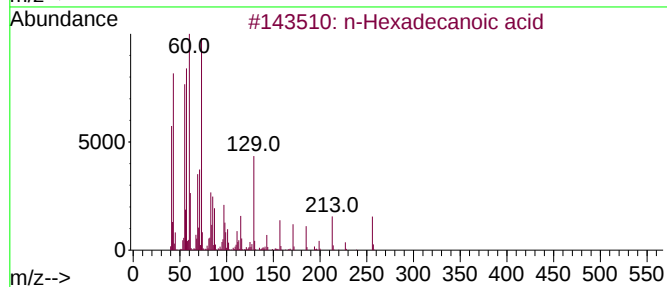
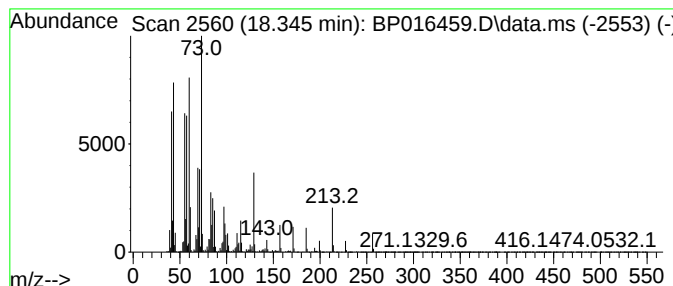
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	20.65 ng	7443730	Phenanthrene-d10	17.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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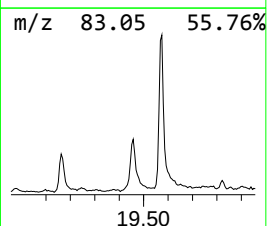
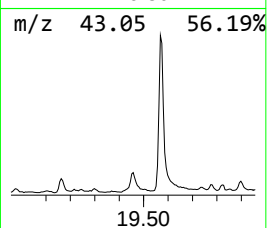
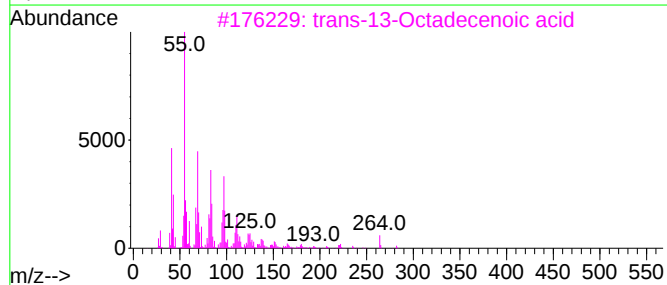
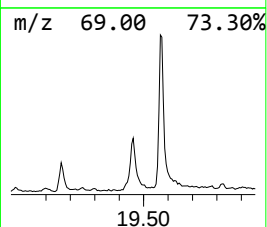
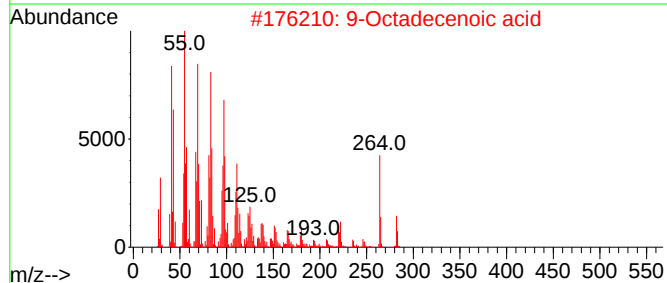
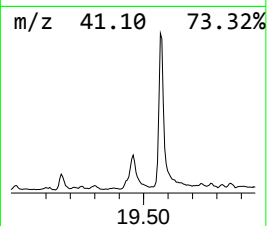
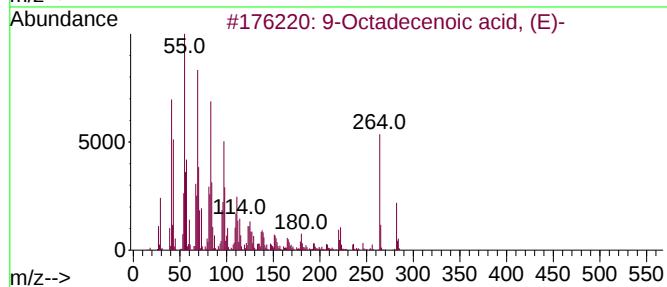
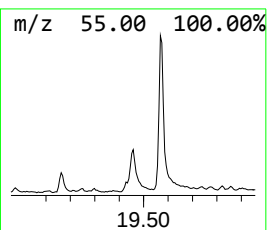
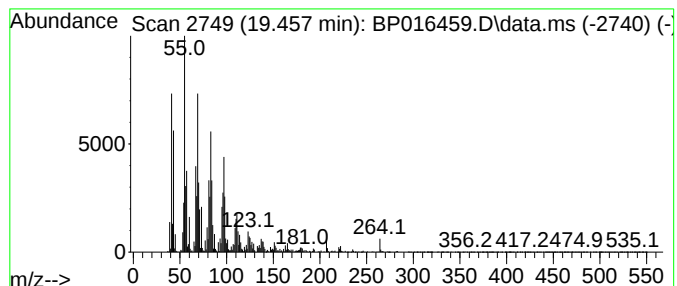
Instrument :
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ClientSampleId :
T842-FH-02-CT

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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 9-Octadecenoic acid, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.457	4.15 ng	1495350	Phenanthrene-d10	17.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	92
2	9-Octadecenoic acid	282	C18H34O2	002027-47-6	90
3	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	81
4	Oleic Acid	282	C18H34O2	000112-80-1	81
5	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016459.D
Acq On : 01 Aug 2023 16:46
Operator : MA/JU
Sample : 03715-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
T842-FH-02-CT

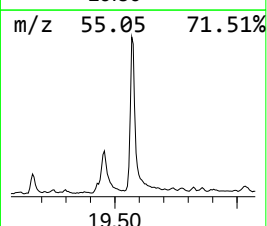
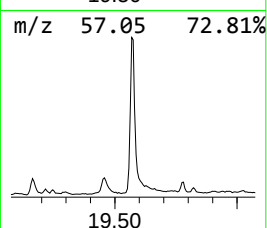
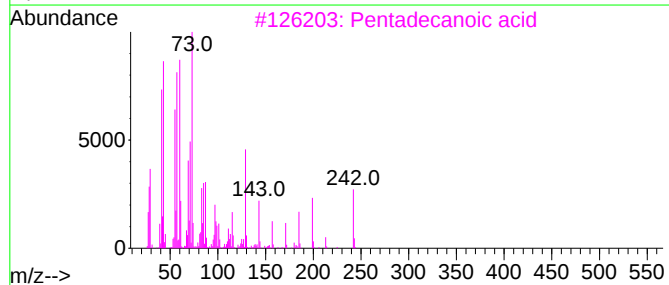
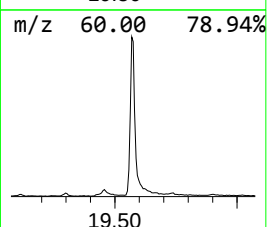
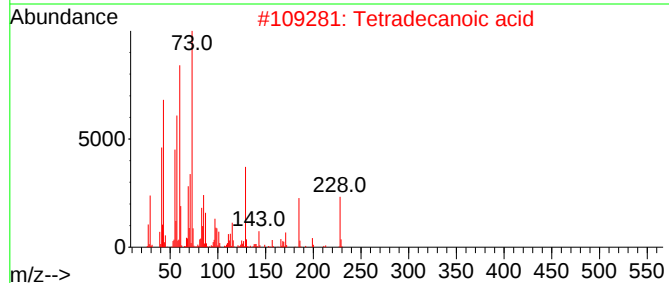
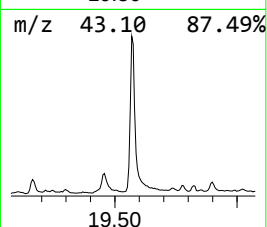
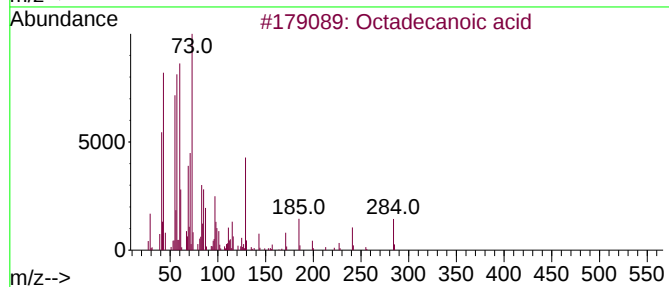
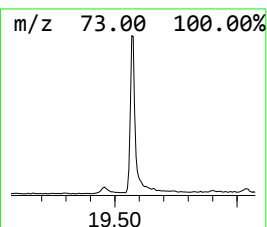
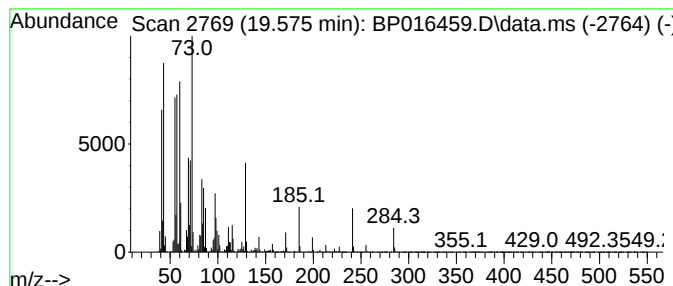
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.575	14.19 ng	4461490	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			n-Decanoic acid	172	C10H20O2	000334-48-5	62
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
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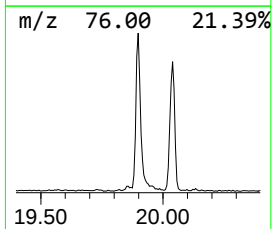
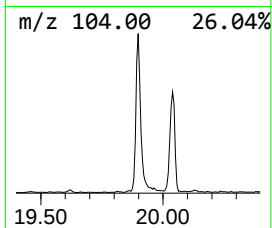
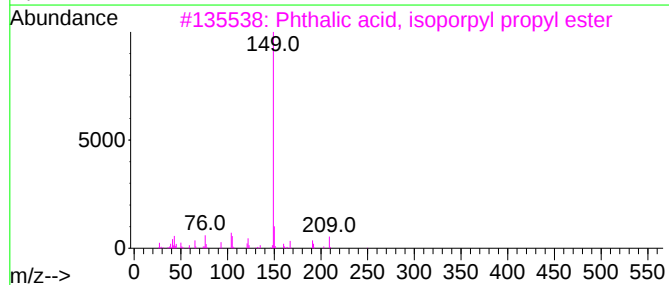
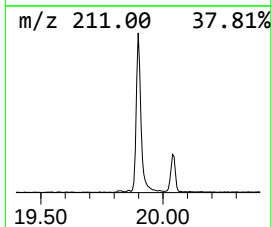
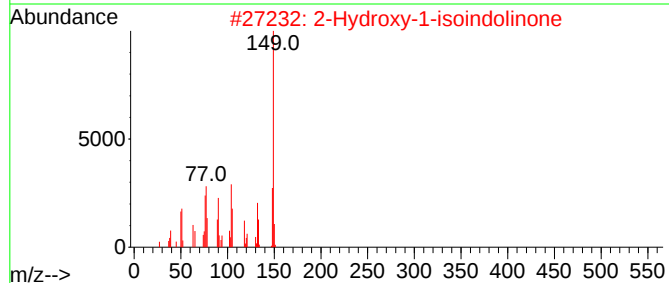
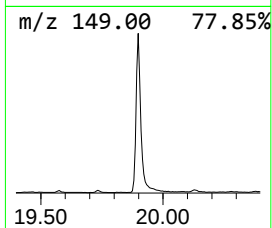
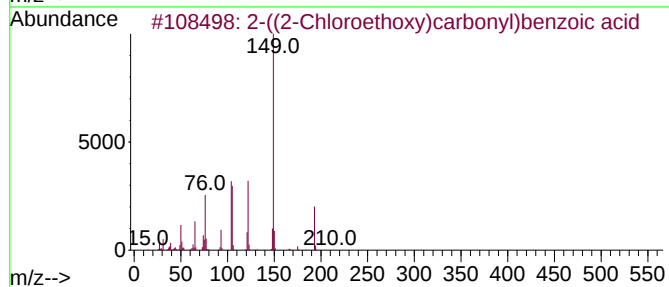
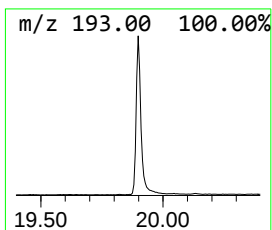
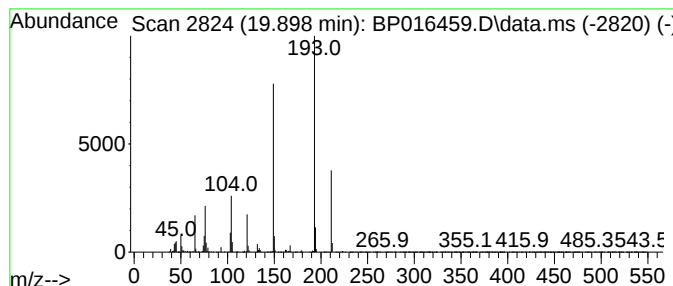
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown19.898 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.898	6.52 ng	2048640	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-((2-Chloroethoxy)carbonyl)benz...	228	C10H9ClO4	006139-60-2	45		
2	2-Hydroxy-1-isoindolinone	149	C8H7NO2	1000289-12-0	38		
3	Phthalic acid, isopropyl propyl ...	250	C14H18O4	1010314-99-7	35		
4	Phthalic acid, ethyl isopropyl e...	236	C13H16O4	1000314-99-6	35		
5	2-((But-3-enyloxy)carbonyl)benzo...	220	C12H12O4	113793-34-3	27		



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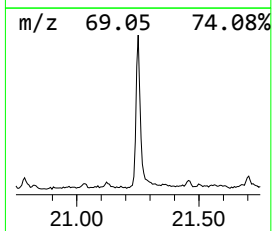
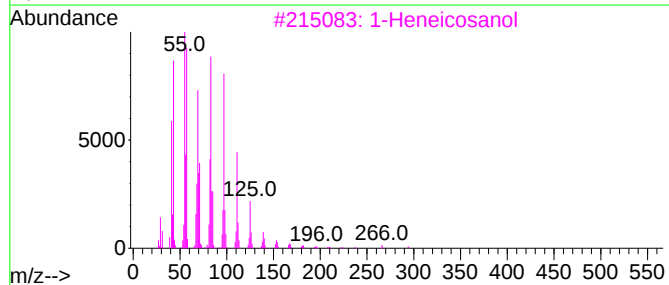
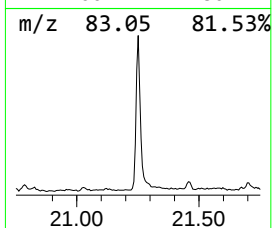
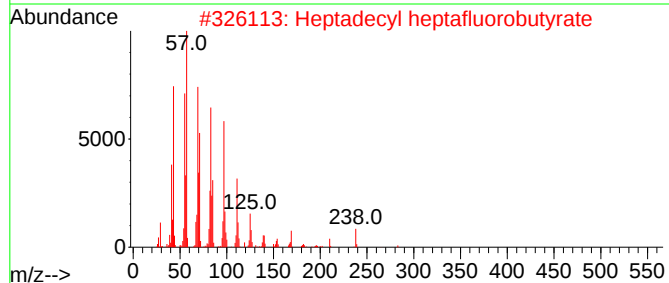
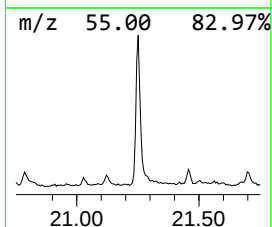
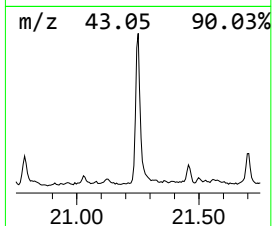
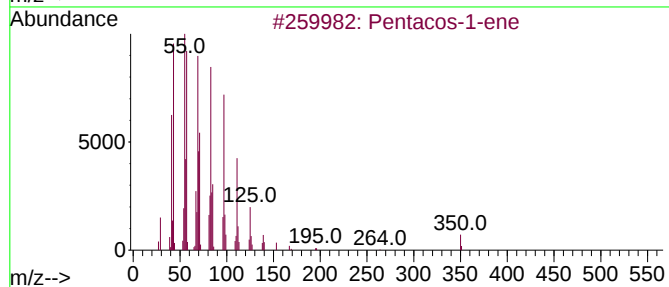
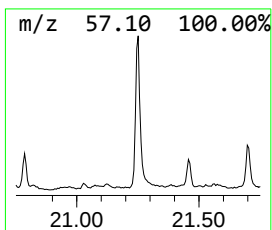
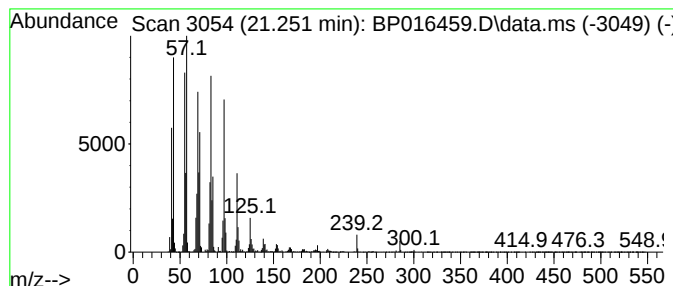
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentacos-1-ene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.251	7.95 ng	2498350	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacos-1-ene	350	C25H50	016980-85-1	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			1-Hexacosanol	382	C26H54O	000506-52-5	91
5			1-Hexacosene	364	C26H52	018835-33-1	91



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Data File : BP016459.D
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ALS Vial : 17 Sample Multiplier: 1

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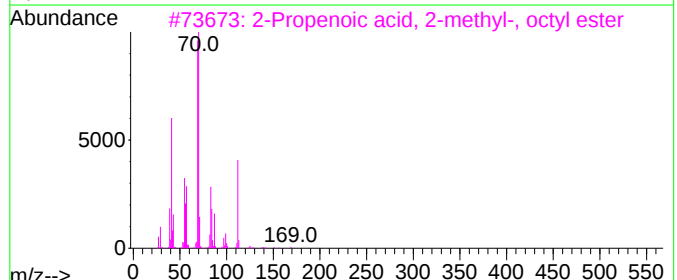
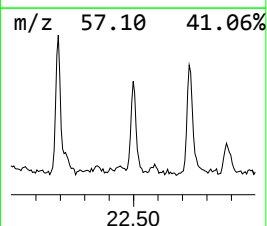
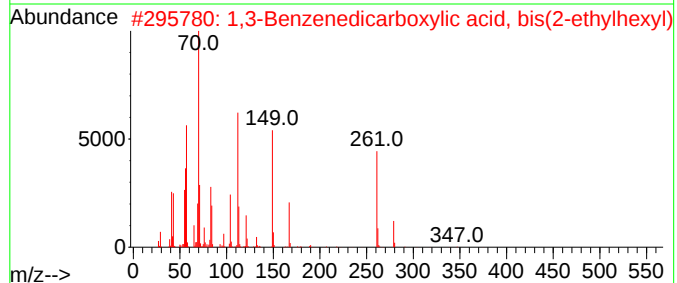
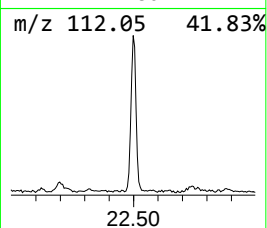
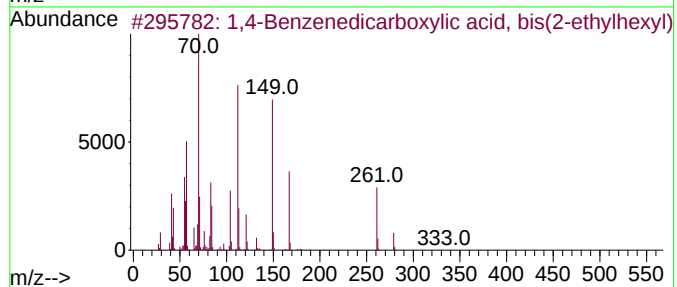
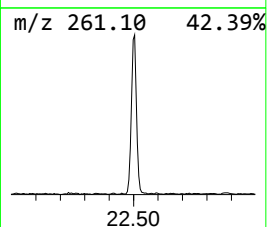
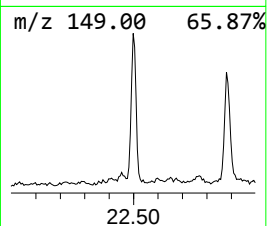
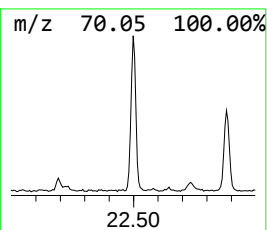
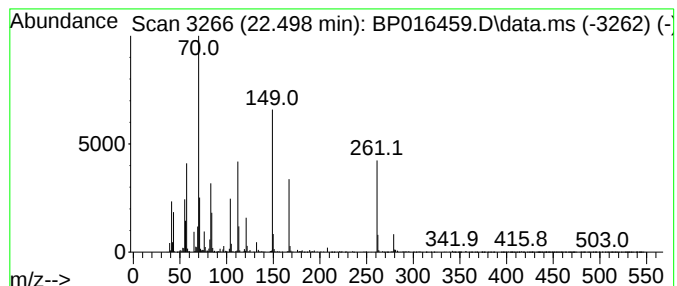
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,4-Benzenedicarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.498	2.38 ng	749715	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	58
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38
3			2-Propenoic acid, 2-methyl-, oct...	198	C12H22O2	002157-01-9	25
4			4-Nitrobenzoic acid, cyclobutyl ...	221	C11H11NO4	070335-00-1	25
5			Phthalic acid, 3,5-difluoropheny...	390	C22H24F2O4	1000315-51-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
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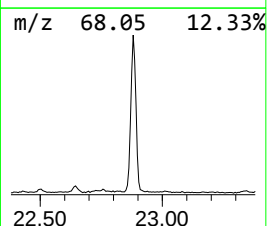
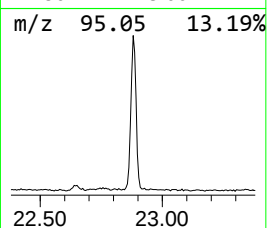
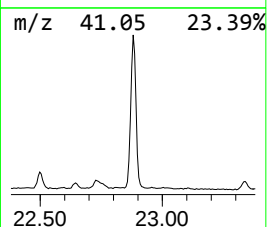
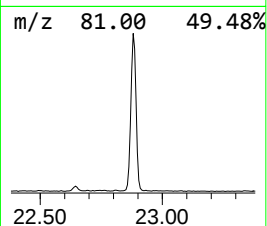
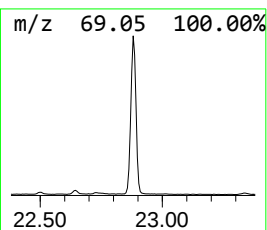
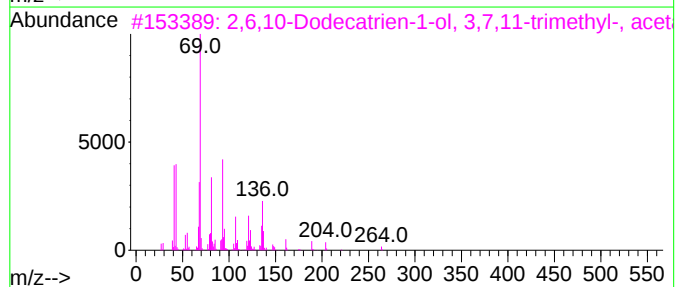
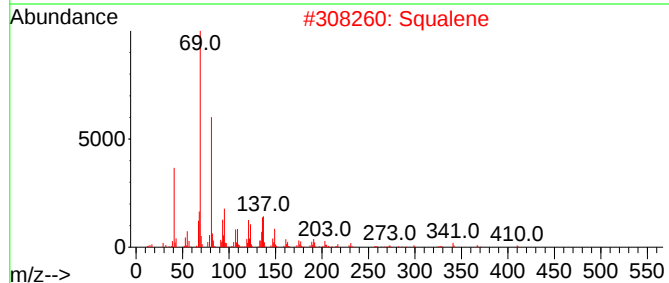
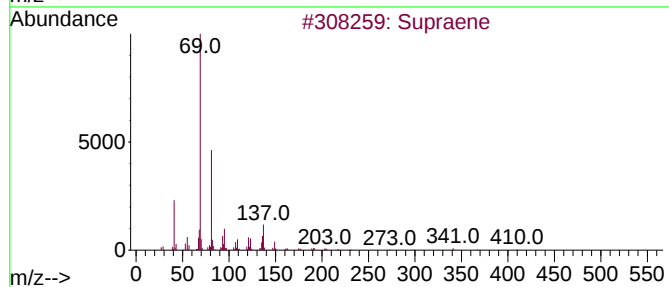
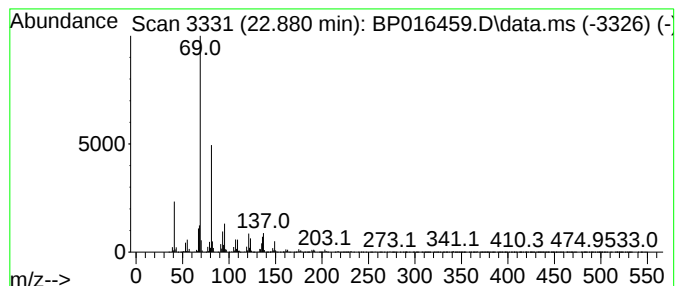
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TIC Integration Parameters: LSCINT.P

Peak Number 10 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.880	12.31 ng	3871370	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
4			Farnesol isomer a	222	C15H26O	1000108-92-4	72
5			Bis(3-methylbut-3-enyl) phthalate	302	C18H22O4	022711-53-1	59



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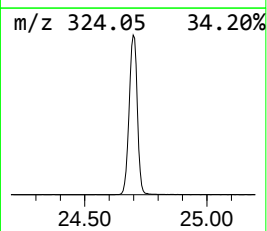
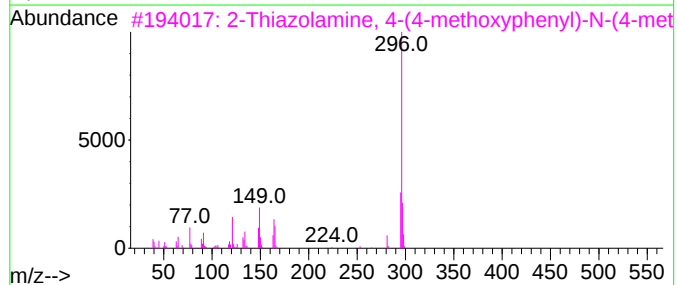
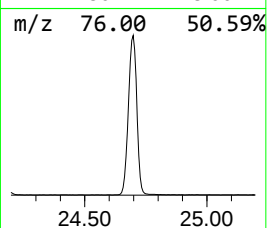
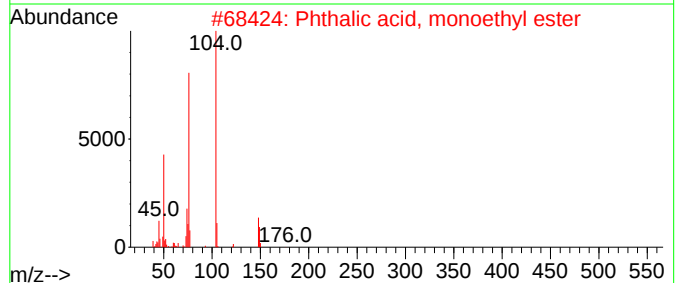
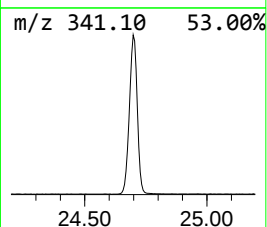
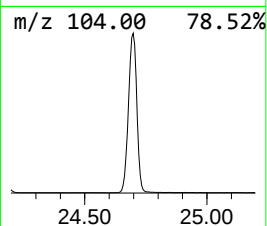
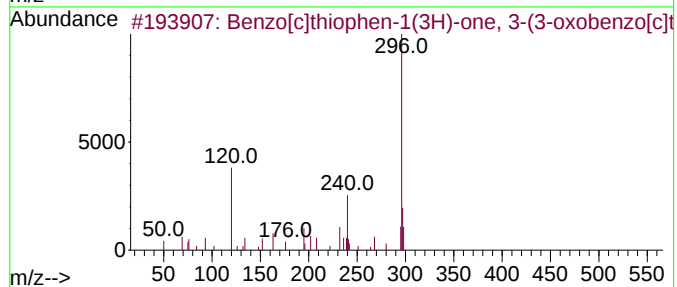
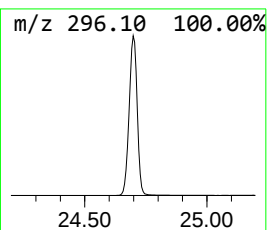
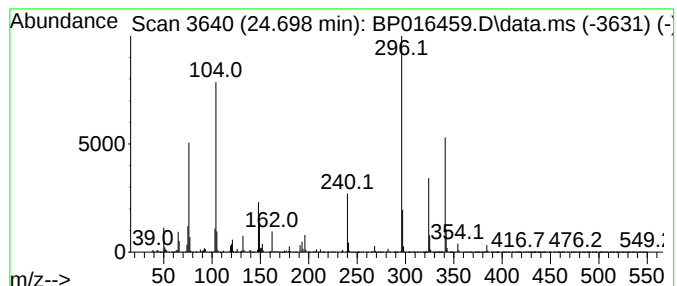
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown24.698 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.698	39.69 ng	11044800	Perylene-d12	24.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophen-1(3H)-one, 3-(3...	296	C16H8O2S2	023667-32-5	22
2			Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	22
3			2-Thiazolamine, 4-(4-methoxyphen...	296	C17H16N2OS	1010319-57-2	18
4			Phthalic anhydride	148	C8H4O3	000085-44-9	16
5			1-Methyl-2,4,6-tris(cyclopentyl)...	296	C22H32	100325-74-4	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
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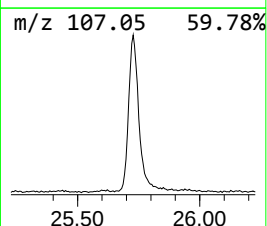
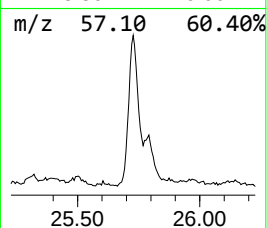
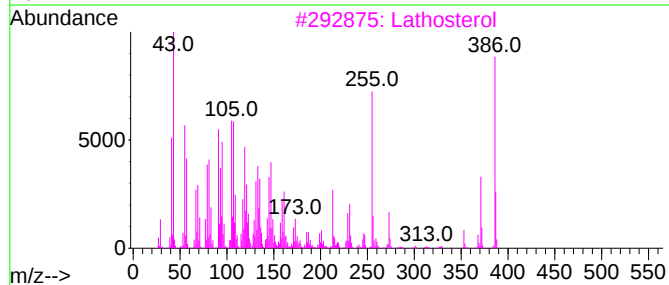
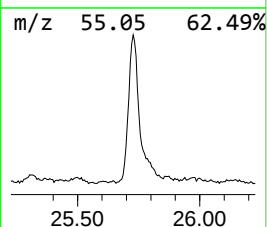
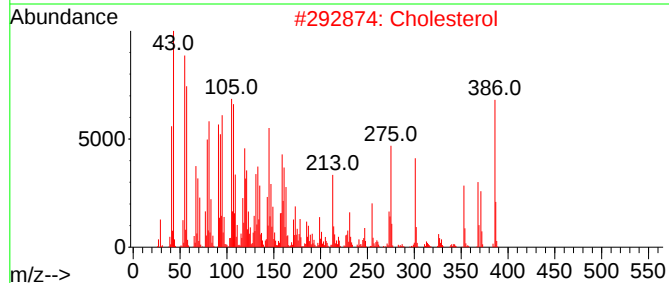
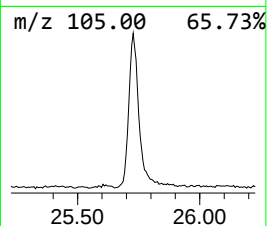
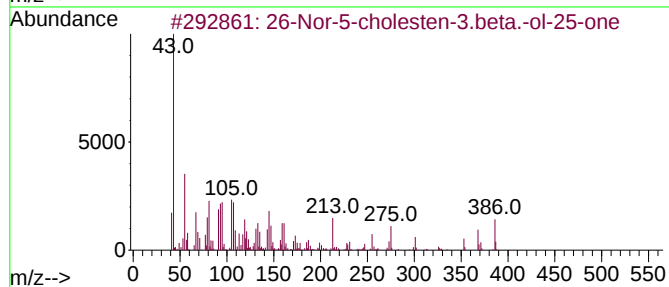
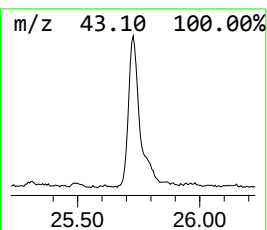
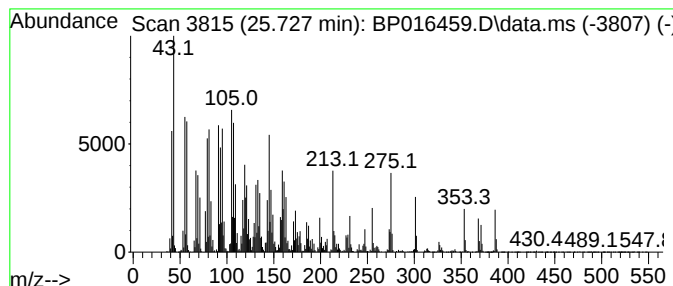
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 26-Nor-5-cholesten-3.beta.-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.727	22.20 ng	6178600	Perylene-d12	24.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99		
2	Cholesterol	386	C27H46O	000057-88-5	99		
3	Lathosterol	386	C27H46O	000080-99-9	92		
4	Cholesterol 3.beta.-O-[2-chloroe...	448	C29H49ClO	001972-30-1	64		
5	Cholestane, 4,5-epoxy-, (4.alpha...	386	C27H46O	006079-19-2	53		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016459.D
Acq On : 01 Aug 2023 16:46
Operator : MA/JU
Sample : 03715-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
T842-FH-02-CT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.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
2-Pentanone, 4-...	5.140	2.3	ng	382526	1	8.075	3266970	20.0
1-Decene	14.339	2.5	ng	770188	3	14.728	6093480	20.0
Benzophenone	16.104	105.4	ng	32113500	3	14.728	6093480	20.0
n-Hexadecanoic ...	18.345	20.6	ng	7443730	4	17.492	7209930	20.0
9-Octadecenoic ...	19.457	4.2	ng	1495350	4	17.492	7209930	20.0
Octadecanoic acid	19.575	14.2	ng	4461490	5	21.586	6288250	20.0
unknown19.898	19.898	6.5	ng	2048640	5	21.586	6288250	20.0
Pentacos-1-ene	21.251	8.0	ng	2498350	5	21.586	6288250	20.0
1,4-Benzenedica...	22.498	2.4	ng	749715	5	21.586	6288250	20.0
Supraene	22.880	12.3	ng	3871370	5	21.586	6288250	20.0
unknown24.698	24.698	39.7	ng	11044800	6	24.186	5565920	20.0
26-Nor-5-choles...	25.727	22.2	ng	6178600	6	24.186	5565920	20.0