

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011823\
 Data File : BF132138.D
 Acq On : 19 Jan 2023 01:56
 Operator : CG\JU
 Sample : 01190-10
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-9

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_F\Methods\8270-BF011823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132138.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.348	419	427	435	rBV	1591576	2101855	40.46%	5.361%
2	5.725	485	491	494	rBV	4260738	4271395	82.23%	10.896%
3	6.707	652	658	661	rBV	3852566	4316165	83.09%	11.010%
4	7.095	720	724	727	rBV	1574246	1226213	23.61%	3.128%
5	7.660	814	820	823	rBV	2912253	2869454	55.24%	7.320%
6	8.383	939	943	946	rBV	1755309	1551256	29.86%	3.957%
7	9.460	1121	1126	1129	rBV	5410382	4869127	93.74%	12.420%
8	10.148	1239	1243	1246	rVB	2011429	1809439	34.83%	4.616%
9	10.860	1361	1364	1367	rBV	640432	464753	8.95%	1.186%
10	10.936	1373	1377	1381	rBV	3501363	3522680	67.82%	8.986%
11	11.642	1493	1497	1501	rBV	2177300	1961619	37.76%	5.004%
12	11.707	1505	1508	1512	rBV2	78736	78659	1.51%	0.201%
13	12.154	1580	1584	1590	rBV	550315	509652	9.81%	1.300%
14	12.866	1700	1705	1707	rBV2	73291	87274	1.68%	0.223%
15	12.942	1715	1718	1726	rBV	126809	132170	2.54%	0.337%
16	13.242	1764	1769	1772	rBV	5563527	5194537	100.00%	13.250%
17	13.430	1794	1801	1804	rBV	58298	78474	1.51%	0.200%
18	14.183	1922	1929	1946	rVB5	88346	332802	6.41%	0.849%
19	14.307	1946	1950	1954	rBV	1700310	1519236	29.25%	3.875%
20	14.395	1959	1965	1972	rBV	410162	448872	8.64%	1.145%
21	14.454	1972	1975	1983	rVB	60776	61798	1.19%	0.158%
22	15.201	2097	2102	2108	rBV	495339	520205	10.01%	1.327%
23	15.907	2216	2222	2230	rBV	932976	1275157	24.55%	3.253%

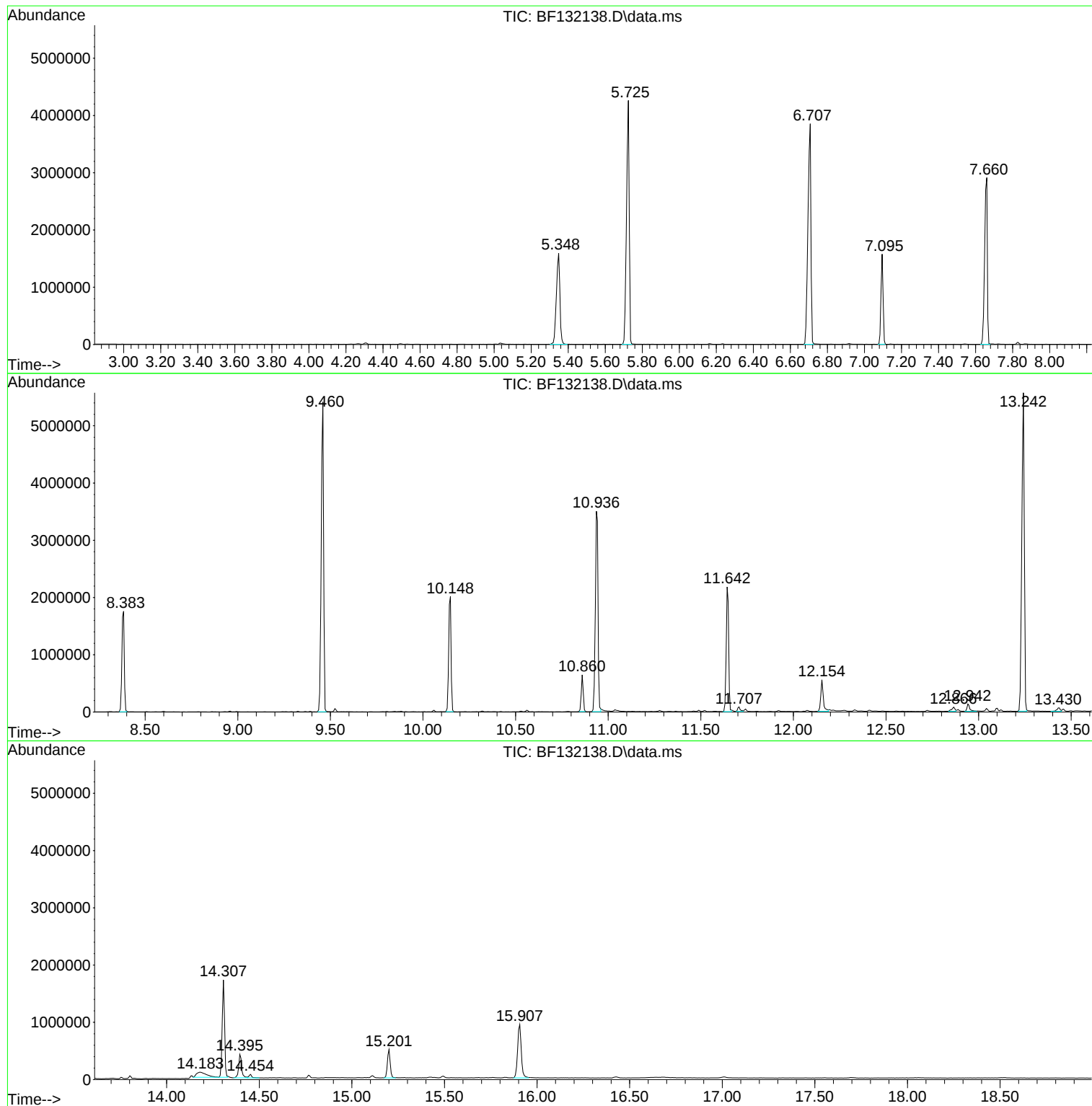
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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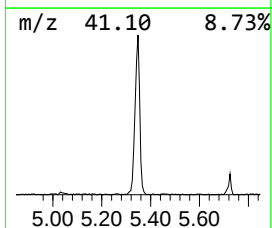
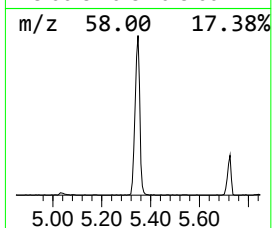
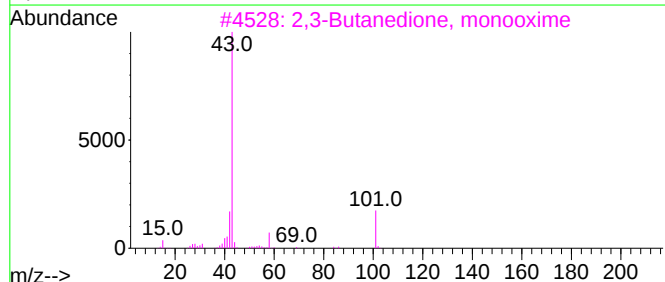
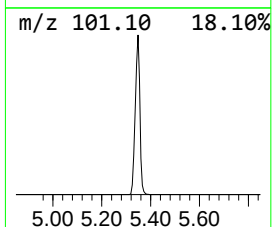
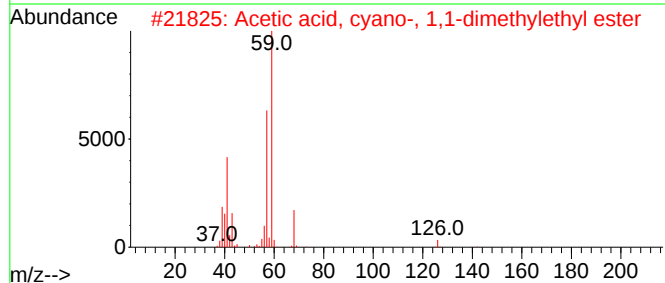
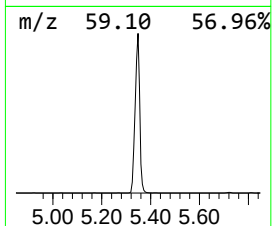
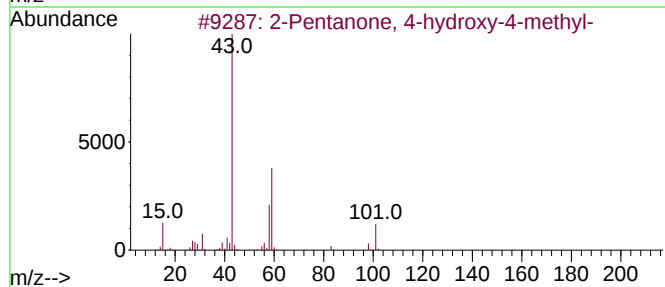
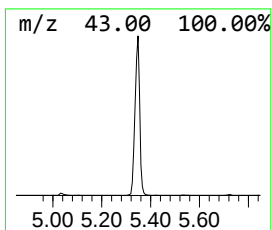
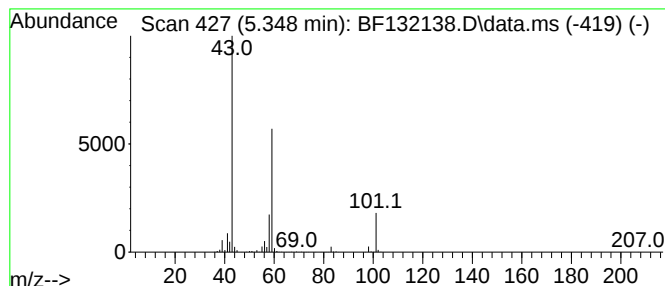
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.348	34.28 ng	2101860	1,4-Dichlorobenzene-d4	7.095

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9



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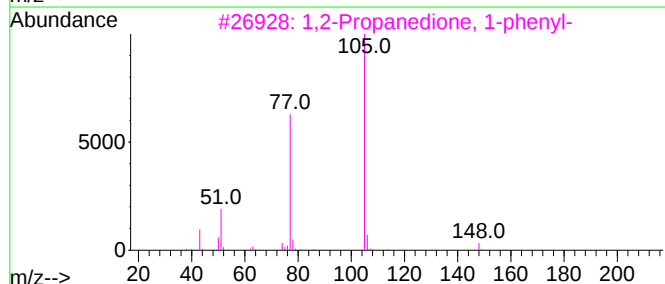
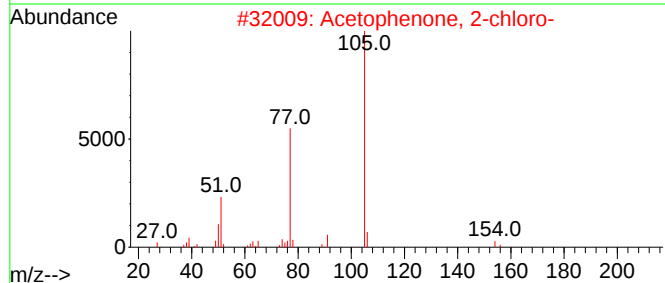
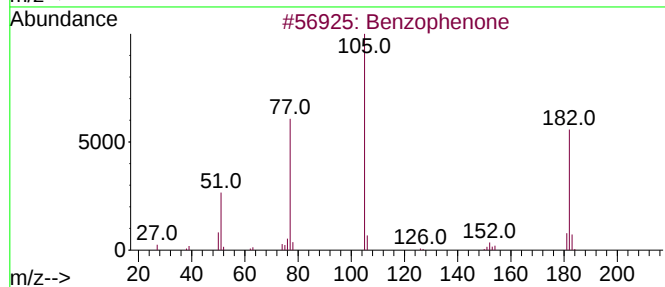
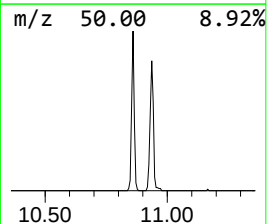
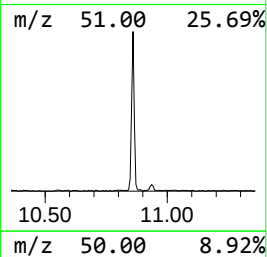
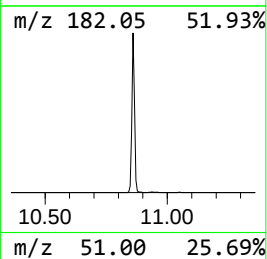
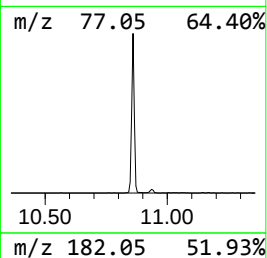
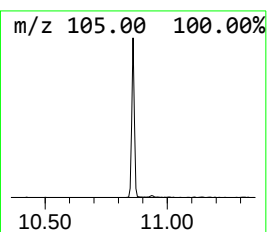
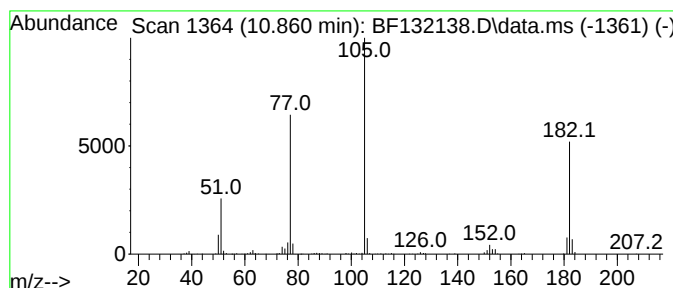
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.860	5.14 ng	464753	Acenaphthene-d10	10.148

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47



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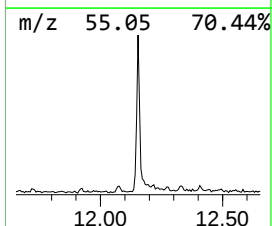
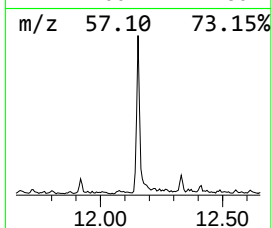
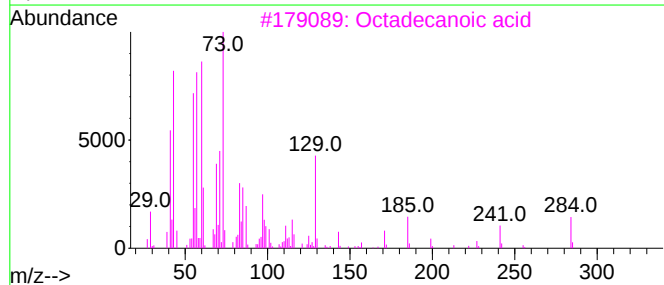
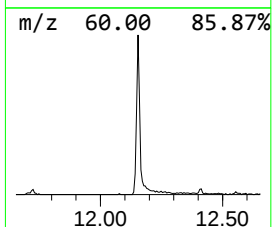
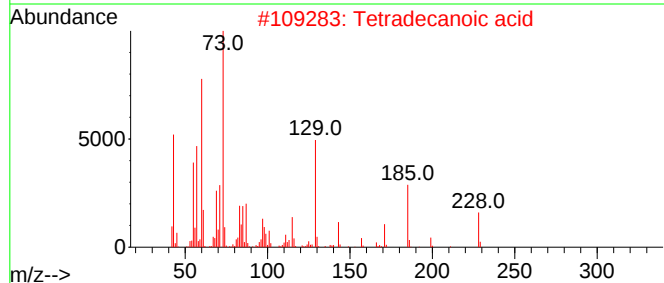
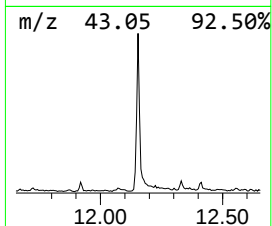
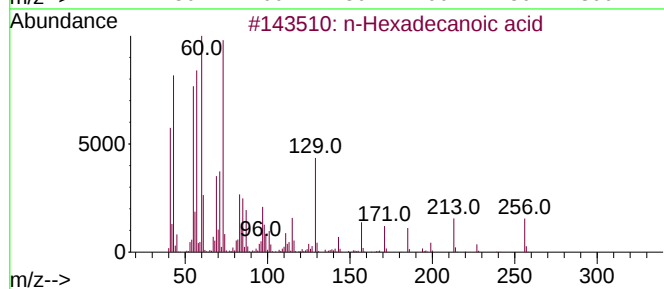
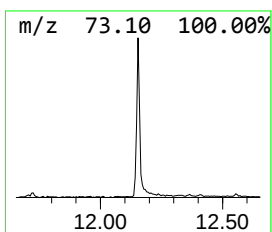
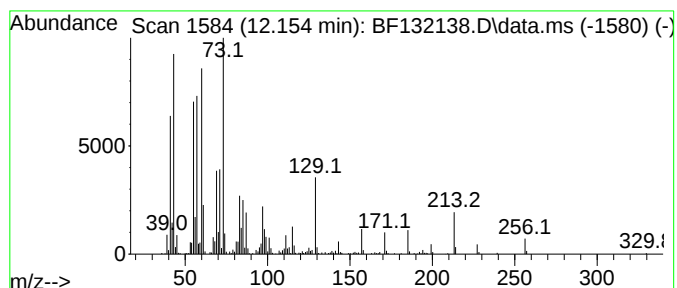
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.154	5.20 ng	509652	Phenanthrene-d10	11.642	
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	91
3	Octadecanoic acid	284	C18H36O2	000057-11-4	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	81



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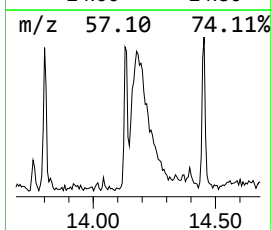
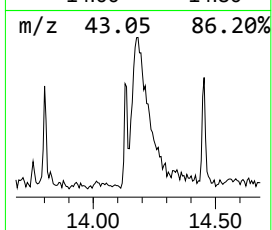
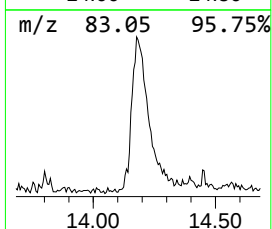
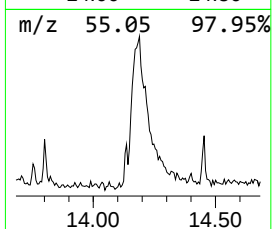
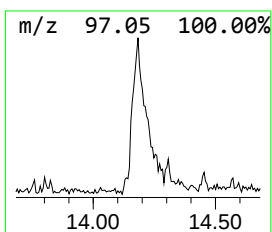
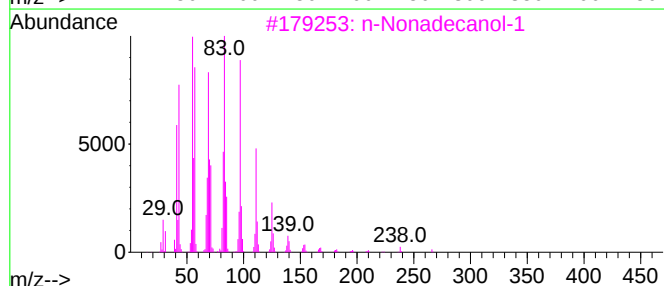
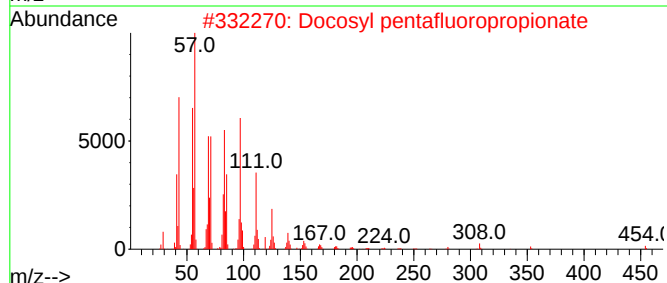
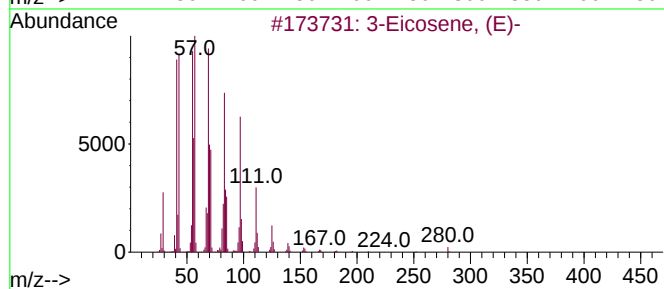
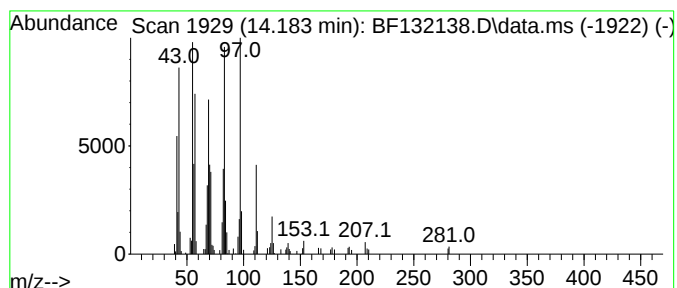
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Peak Number 4 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.183	4.38 ng	332802	Chrysene-d12	14.307	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
4	1-Octadecanol	270	C18H38O	000112-92-5	87
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	83



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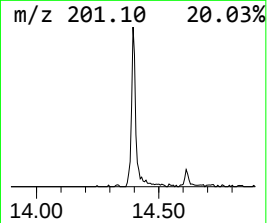
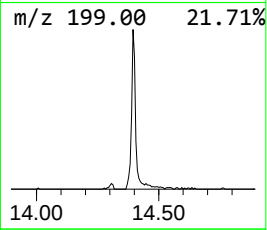
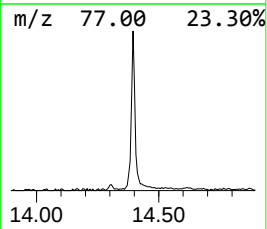
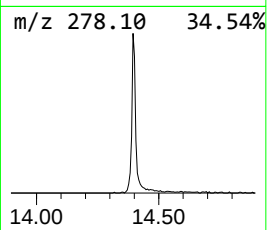
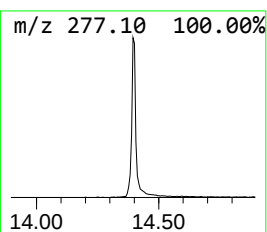
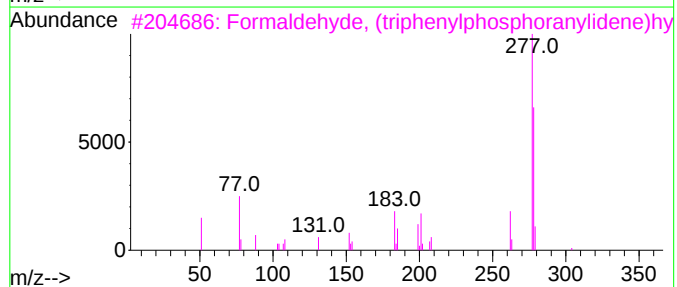
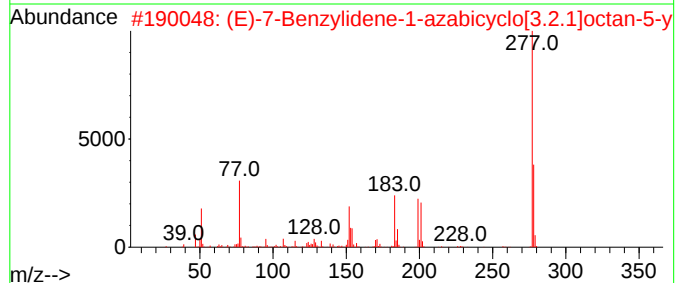
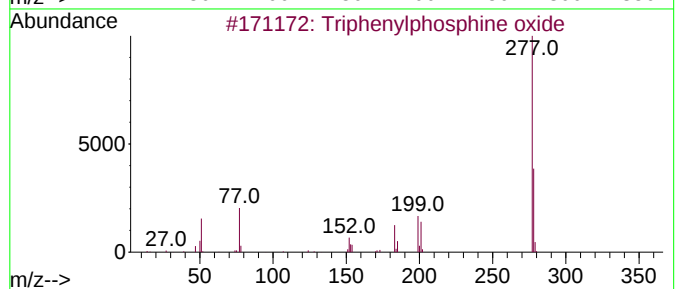
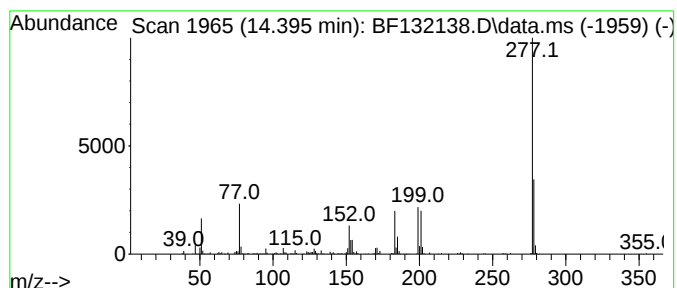
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.395	5.91 ng	448872	Chrysene-d12	14.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	32



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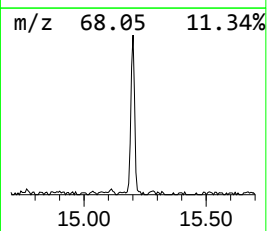
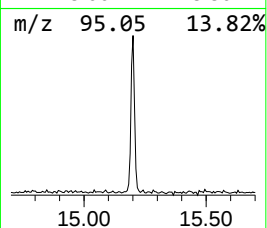
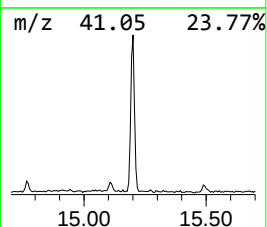
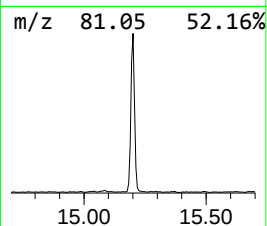
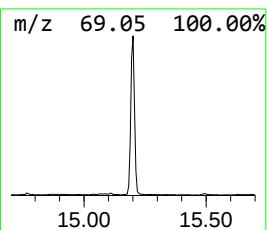
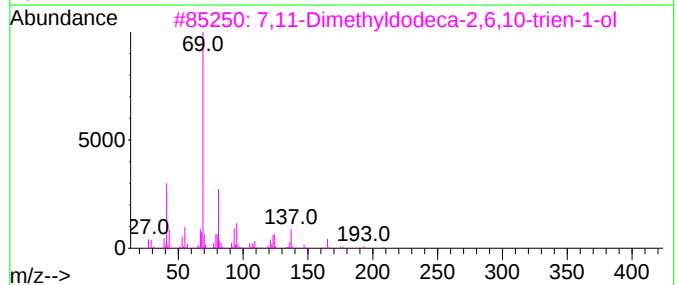
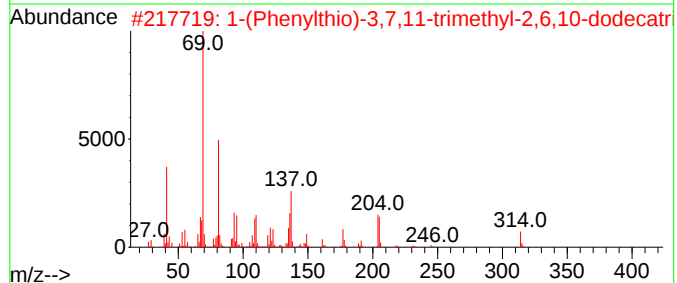
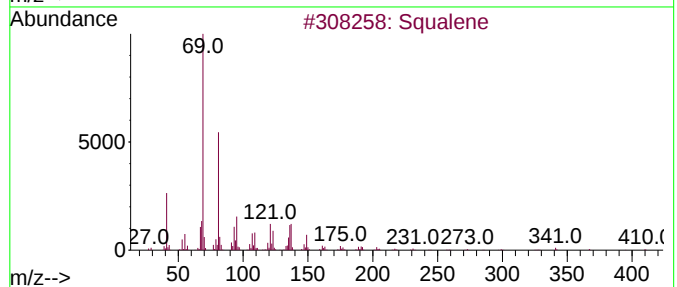
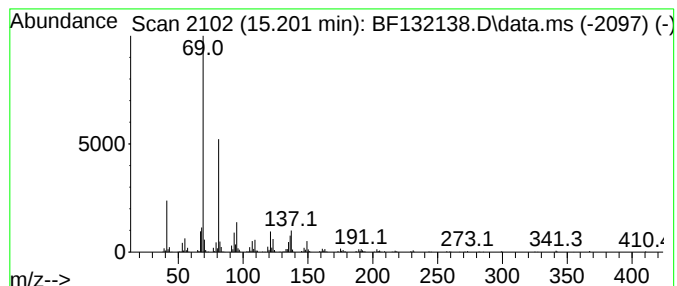
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.201	8.16 ng	520205	Perylene-d12	15.906

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	96
2			1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	78
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
5			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011823\
Data File : BF132138.D
Acq On : 19 Jan 2023 01:56
Operator : CG\JU
Sample : 01190-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011823.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
2-Pentanone, 4-...	5.348	34.3	ng	2101860	1	7.095	1226210	20.0
Benzophenone	10.860	5.1	ng	464753	3	10.148	1809440	20.0
n-Hexadecanoic ...	12.154	5.2	ng	509652	4	11.642	1961620	20.0
3-Eicosene, (E)-	14.183	4.4	ng	332802	5	14.307	1519240	20.0
Triphenylphosph...	14.395	5.9	ng	448872	5	14.307	1519240	20.0
Squalene	15.201	8.2	ng	520205	6	15.906	1275160	20.0