

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090122\
 Data File : BF130082.D
 Acq On : 01 Sep 2022 17:36
 Operator : CG\JU
 Sample : N4383-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 252672-1

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-BF083122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130082.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.710	67	72	81	rVB	104034	163000	2.07%	0.383%
2	4.904	441	445	454	rBV	181967	223223	2.83%	0.525%
3	5.310	509	514	517	rBV	3645924	3418117	43.37%	8.041%
4	6.328	682	687	690	rBV	2876113	2614276	33.17%	6.150%
5	6.704	747	751	754	rBV	1543654	1298523	16.48%	3.055%
6	7.269	841	847	850	rBV	3992169	4341630	55.09%	10.213%
7	7.981	964	968	972	rBV	1958391	1766365	22.41%	4.155%
8	9.063	1146	1152	1155	rBV	7417389	7880794	100.00%	18.539%
9	9.733	1261	1266	1269	rBV	2392206	2001986	25.40%	4.709%
10	10.522	1394	1400	1403	rBV	4811533	4851335	61.56%	11.412%
11	11.216	1514	1518	1521	rBV	2190203	1893190	24.02%	4.454%
12	11.574	1571	1579	1583	rBV3	39431	106051	1.35%	0.249%
13	11.616	1583	1586	1590	rVB	366291	321717	4.08%	0.757%
14	11.751	1605	1609	1613	rBV2	106731	122751	1.56%	0.289%
15	12.321	1703	1706	1712	rVB	727352	595241	7.55%	1.400%
16	12.380	1712	1716	1718	rBV2	66283	101106	1.28%	0.238%
17	12.410	1718	1721	1726	rVV	432634	405856	5.15%	0.955%
18	12.469	1728	1731	1734	rVB	404171	317310	4.03%	0.746%
19	12.810	1783	1789	1792	rBV	6414953	7105047	90.16%	16.714%
20	13.845	1956	1965	1968	rBV	1606044	1564867	19.86%	3.681%
21	13.945	1977	1982	1991	rVB	132183	173384	2.20%	0.408%
22	15.245	2198	2203	2208	rBV	1123319	1244004	15.79%	2.926%

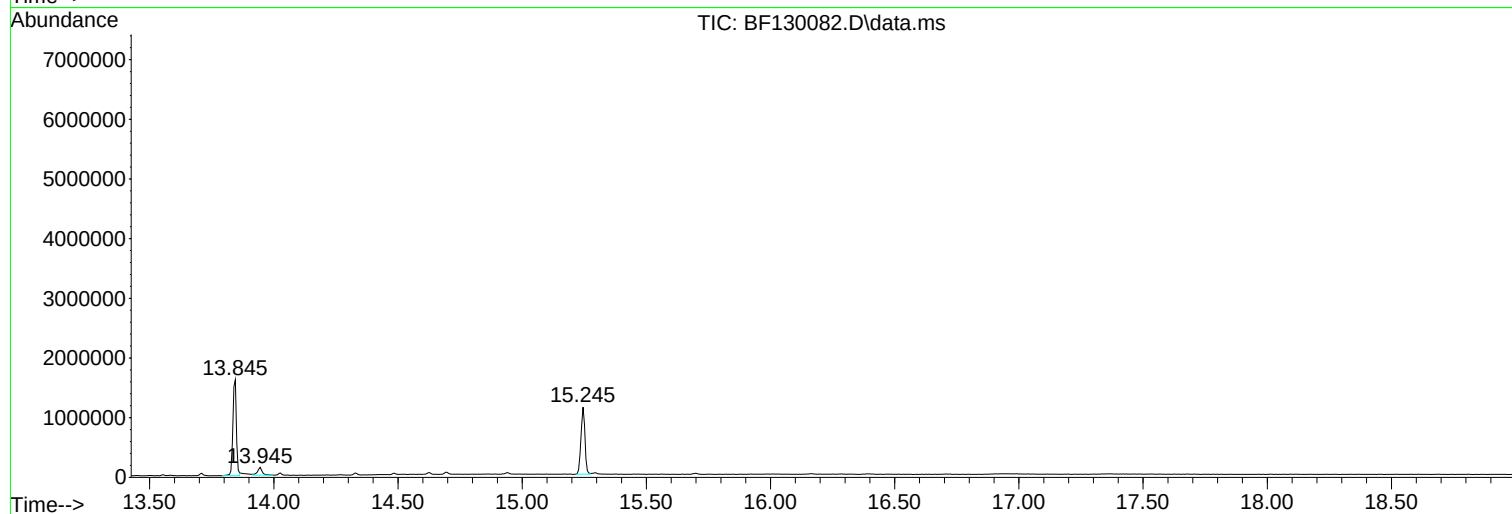
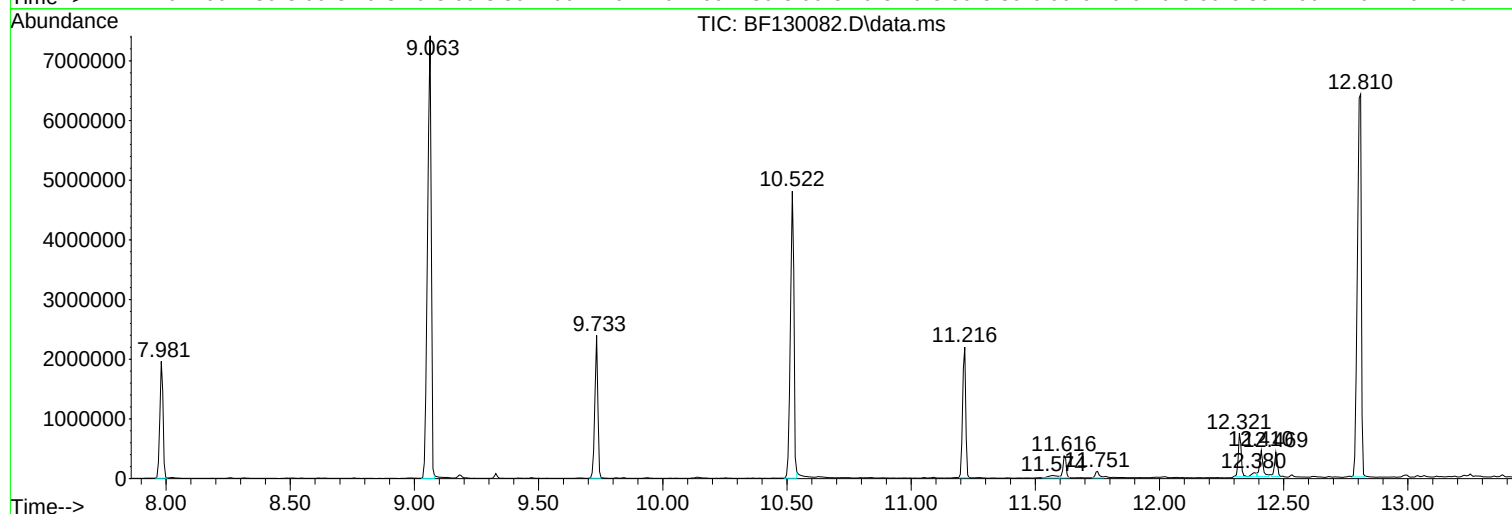
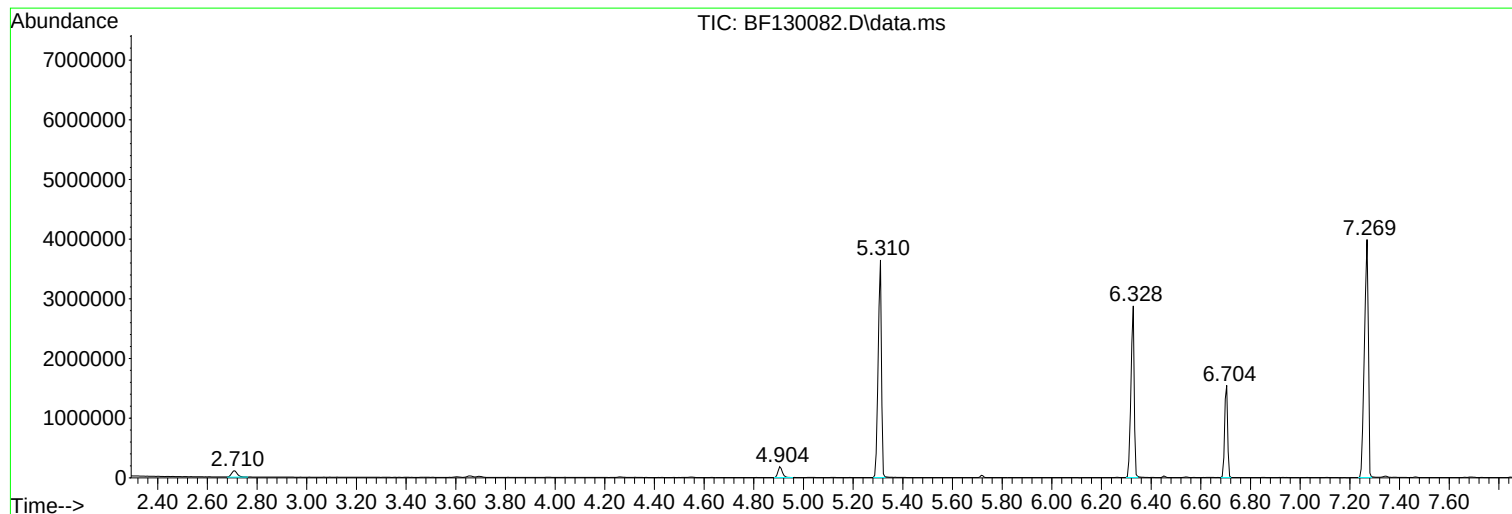
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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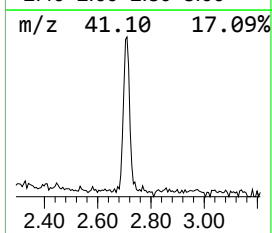
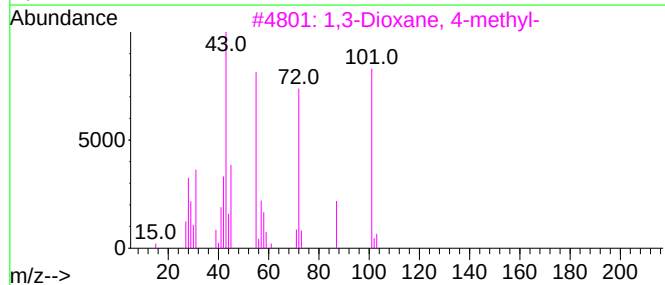
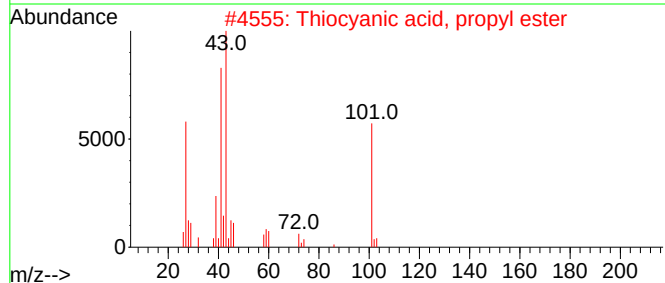
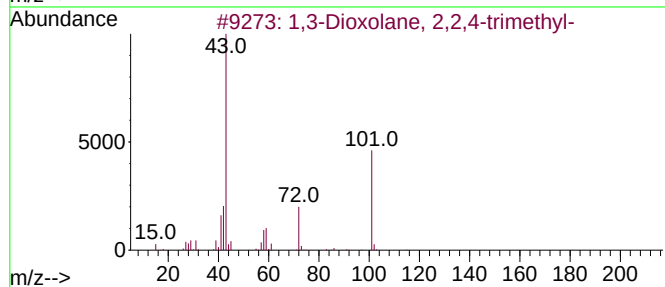
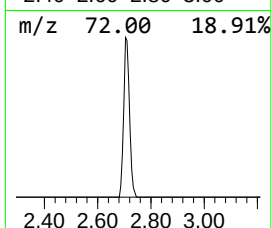
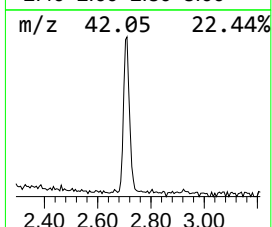
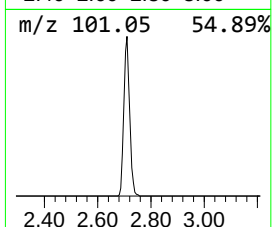
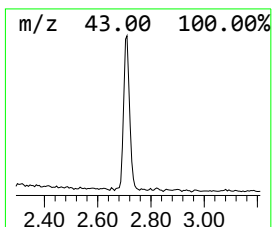
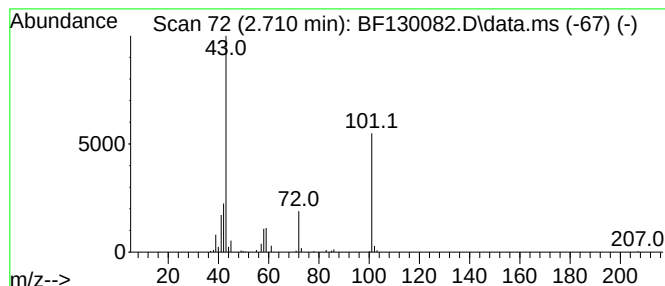
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.710	2.51 ng	163000	1,4-Dichlorobenzene-d4	6.704

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2		Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	59
3		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	59
4		Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	42
5		Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	38



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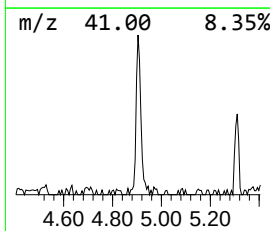
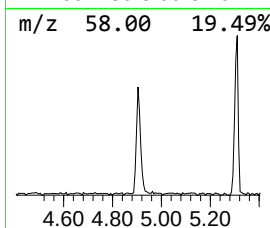
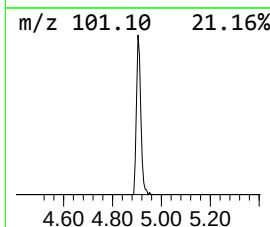
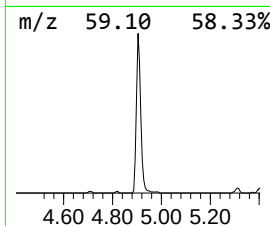
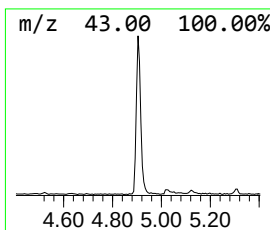
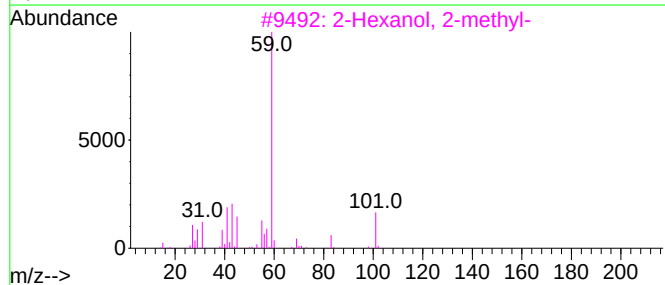
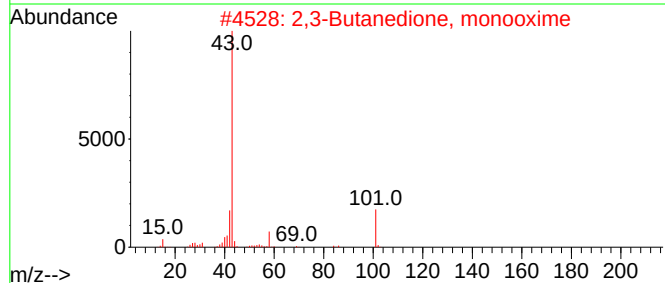
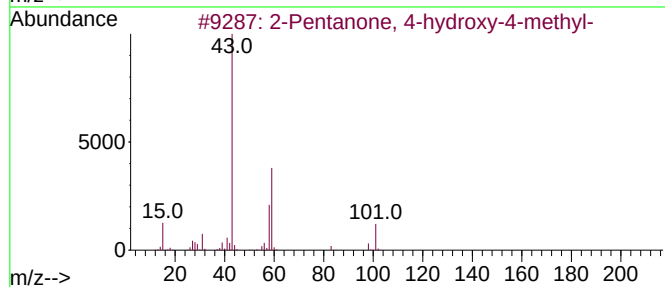
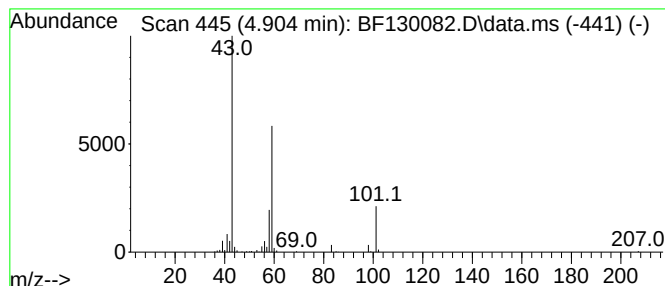
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	3.44 ng	223223	1,4-Dichlorobenzene-d4	6.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	17
4			Acetone	58	C3H6O	000067-64-1	12
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12



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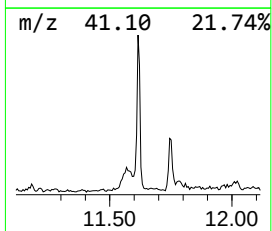
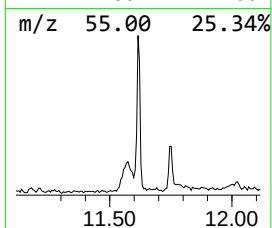
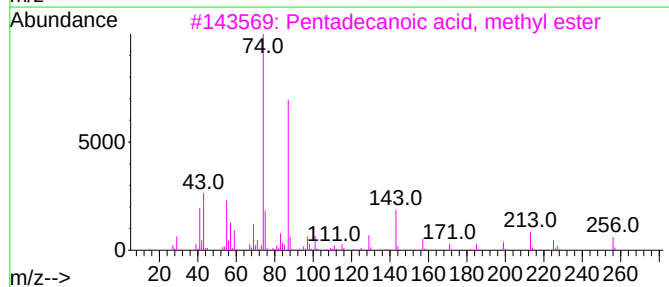
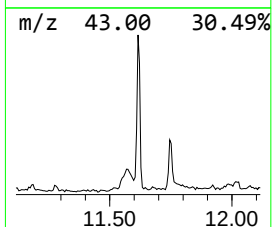
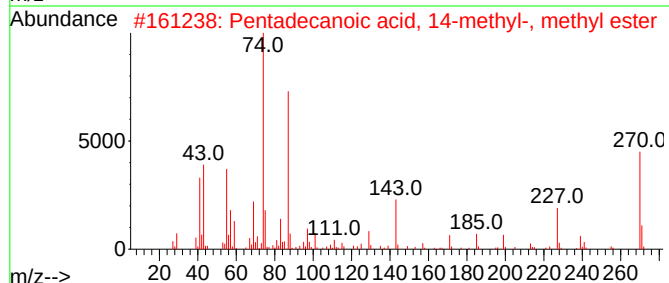
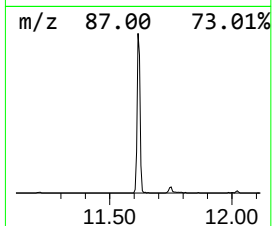
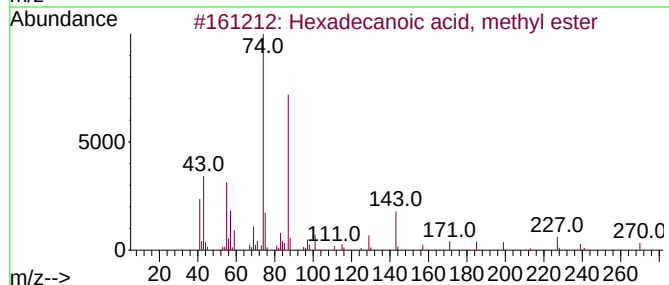
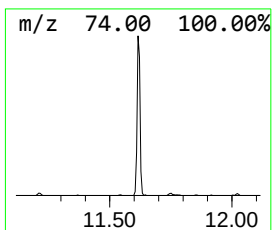
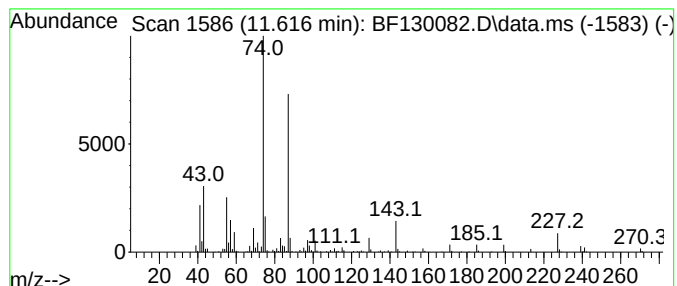
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Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.616	3.40 ng	321717	Phenanthrene-d10		11.216	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...		270	C17H34O2	005129-60-2	94
3	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	90
4	Methyl tetradecanoate		242	C15H30O2	000124-10-7	90
5	Dodecanoic acid, methyl ester		214	C13H26O2	000111-82-0	90



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ALS Vial : 4 Sample Multiplier: 1

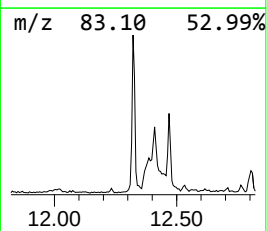
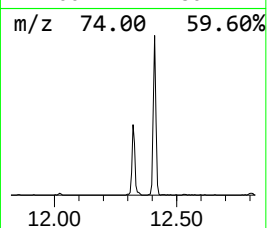
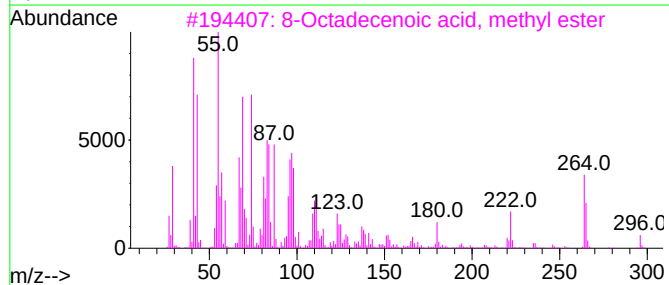
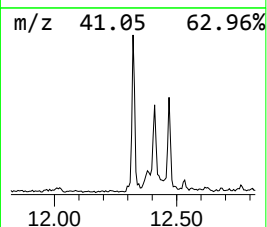
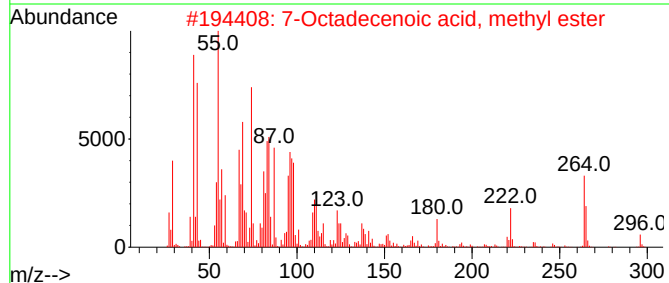
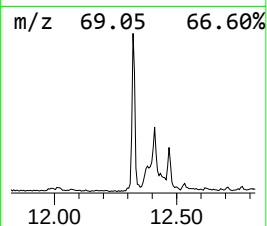
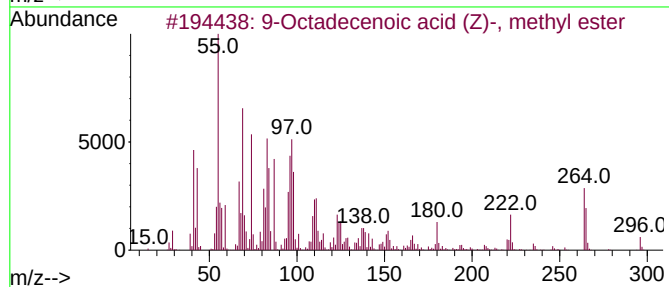
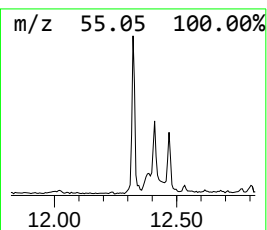
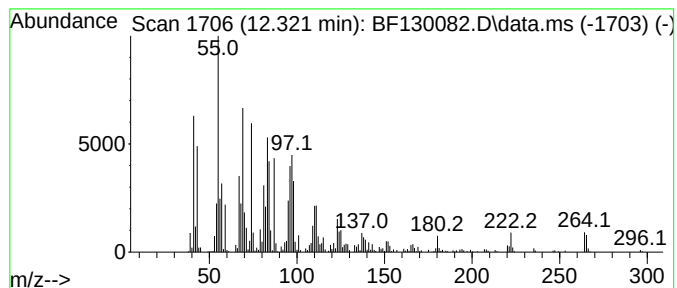
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.322	6.29 ng	595241	Phenanthrene-d10		11.216	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...		296	C19H36O2	000112-62-9	99
2	7-Octadecenoic acid, methyl ester		296	C19H36O2	057396-98-2	99
3	8-Octadecenoic acid, methyl ester		296	C19H36O2	002345-29-1	99
4	9-Octadecenoic acid, methyl este...		296	C19H36O2	001937-62-8	99
5	11-Octadecenoic acid, methyl ester		296	C19H36O2	052380-33-3	99



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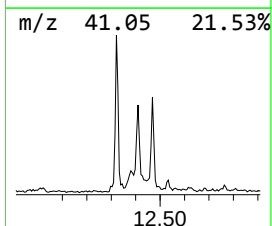
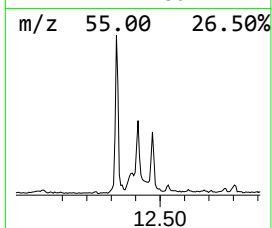
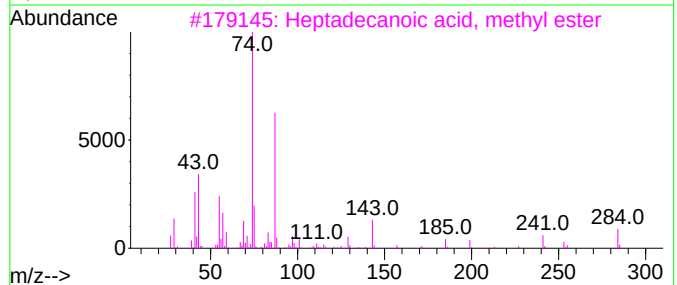
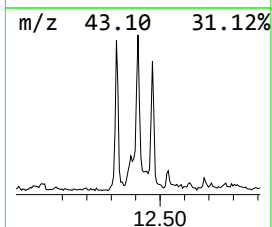
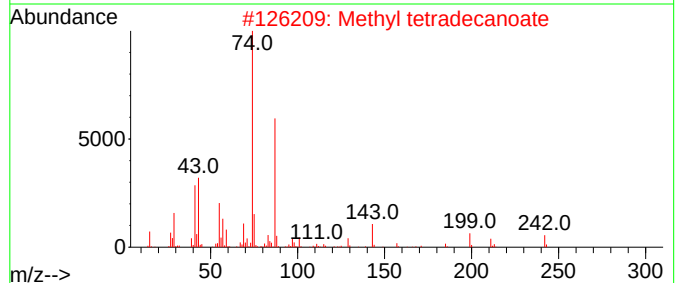
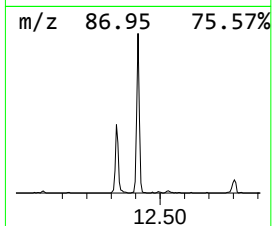
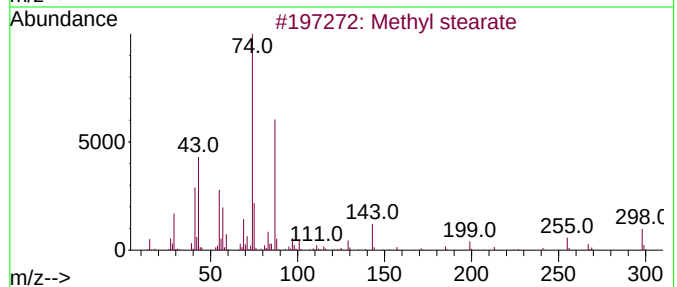
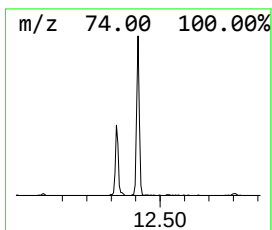
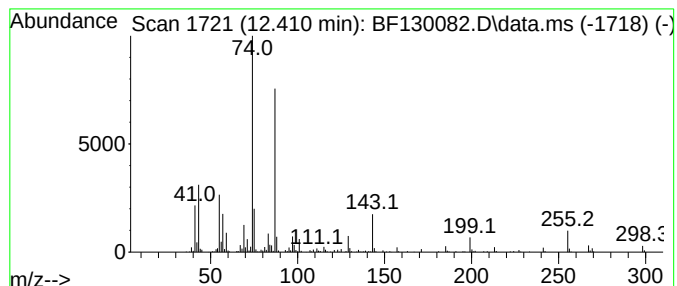
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Methyl stearate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	4.29 ng	405856	Phenanthrene-d10	11.216

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	94
3			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
4			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90



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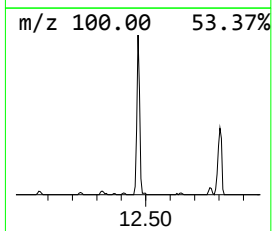
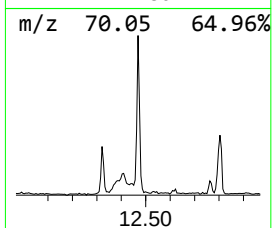
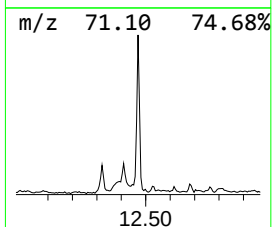
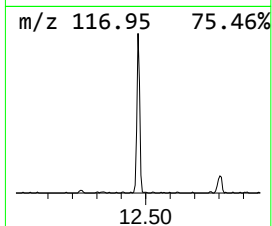
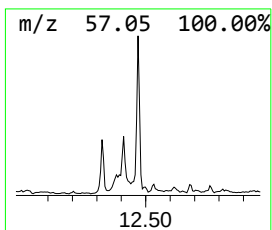
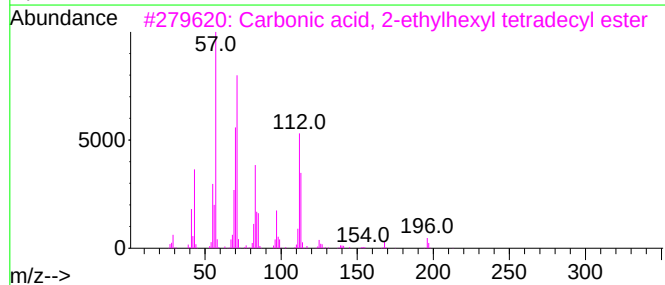
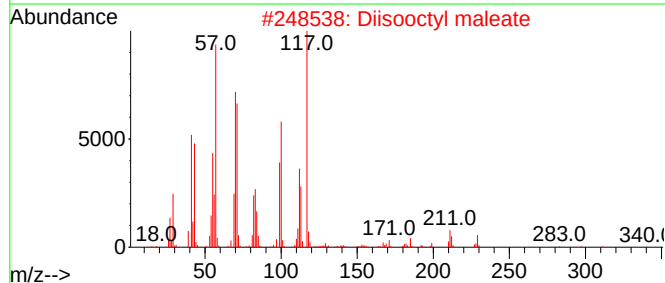
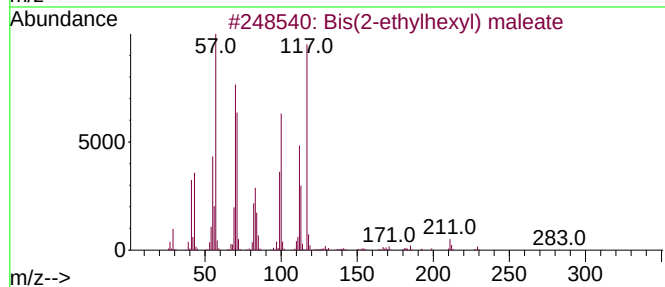
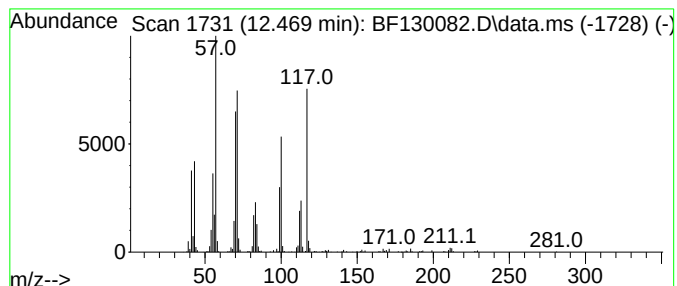
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Bis(2-ethylhexyl) maleate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	3.35 ng	317310	Phenanthrene-d10	11.216

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	91
2			Diisooctyl maleate	340	C20H36O4	001330-76-3	72
3			Carbonic acid, 2-ethylhexyl tetr...	370	C23H46O3	1010383-14-1	38
4			Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	38
5			Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090122\
Data File : BF130082.D
Acq On : 01 Sep 2022 17:36
Operator : CG\JU
Sample : N4383-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
252672-1

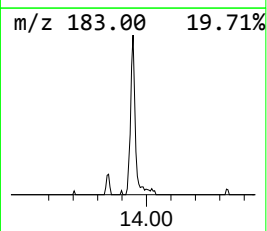
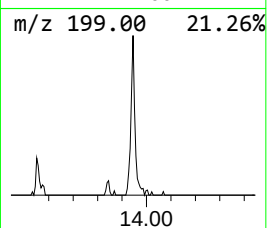
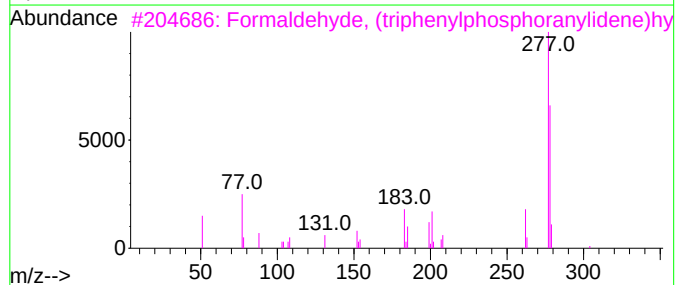
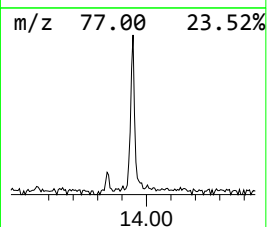
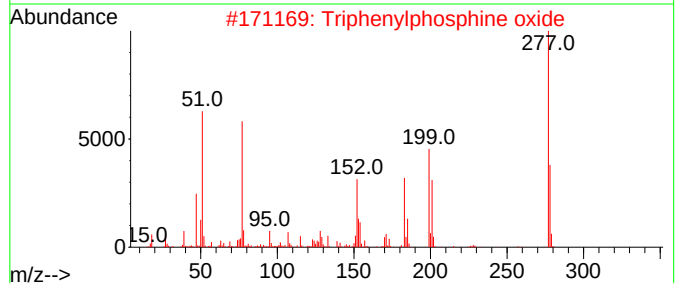
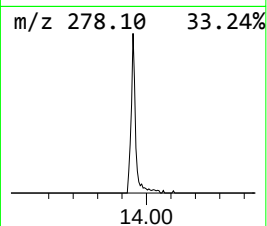
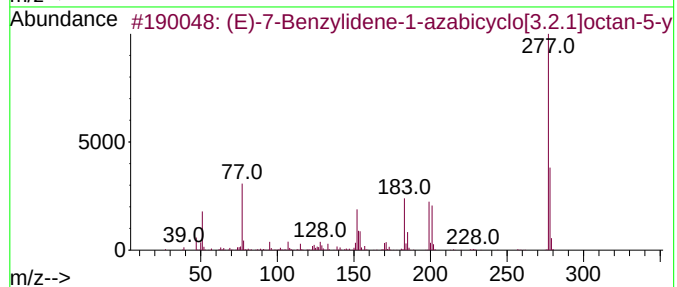
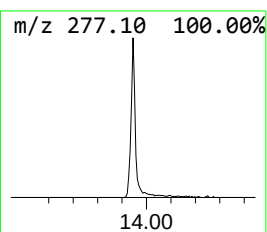
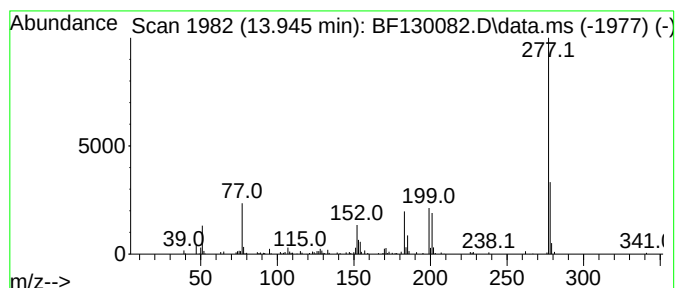
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	2.22 ng	173384	Chrysene-d12	13.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	86		
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64		
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50		
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090122\
Data File : BF130082.D
Acq On : 01 Sep 2022 17:36
Operator : CG\JU
Sample : N4383-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
252672-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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
1,3-Dioxolane, ...	2.710	2.5	ng	163000	1	6.704	1298520	20.0
2-Pentanone, 4-...	4.904	3.4	ng	223223	1	6.704	1298520	20.0
Hexadecanoic ac...	11.616	3.4	ng	321717	4	11.216	1893190	20.0
9-Octadecenoic ...	12.322	6.3	ng	595241	4	11.216	1893190	20.0
Methyl stearate	12.410	4.3	ng	405856	4	11.216	1893190	20.0
Bis(2-ethylhexy...	12.469	3.4	ng	317310	4	11.216	1893190	20.0
(E)-7-Benzylide...	13.945	2.2	ng	173384	5	13.845	1564870	20.0