

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091820\
 Data File : BP003332.D
 Acq On : 18 Sep 2020 21:05
 Operator : CG/JU
 Sample : L3871-13 2X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TR-05-091720

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003332.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.217	390	396	411	rBV	1075820	1614133	10.31%	2.550%
2	6.799	656	665	679	rBV	975355	1641261	10.49%	2.593%
3	7.605	794	802	813	rBV	774252	1240041	7.92%	1.959%
4	8.752	987	997	1010	rBV	654918	1156014	7.39%	1.826%
5	10.381	1265	1274	1292	rBV	993155	1772287	11.32%	2.800%
6	12.869	1690	1697	1716	rBV	1743182	2686006	17.16%	4.243%
7	13.710	1835	1840	1846	rBV	247968	350834	2.24%	0.554%
8	14.251	1925	1932	1945	rBV	1445352	2160840	13.80%	3.413%
9	15.751	2181	2187	2199	rBV	1009080	1567731	10.02%	2.476%
10	17.004	2395	2400	2406	rBV	1428280	2032469	12.98%	3.211%
11	17.704	2514	2519	2524	rBV	4520578	5915263	37.79%	9.344%
12	18.822	2702	2709	2711	rBV	10911021	15653068	100.00%	24.726%
13	18.851	2711	2714	2723	rVV2	9092877	13251986	84.66%	20.933%
14	18.922	2723	2726	2730	rVB2	170954	192389	1.23%	0.304%
15	18.975	2730	2735	2740	rVB	3080142	3534074	22.58%	5.583%
16	19.328	2790	2795	2800	rBV2	222938	305222	1.95%	0.482%
17	19.586	2834	2839	2843	rBV	2119942	2522944	16.12%	3.985%
18	19.933	2895	2898	2909	rVB2	320155	445337	2.85%	0.703%
19	20.039	2912	2916	2919	rBV	327795	394974	2.52%	0.624%
20	20.192	2939	2942	2948	rBV3	331996	411894	2.63%	0.651%
21	20.639	3013	3018	3022	rBV3	243585	442684	2.83%	0.699%
22	20.963	3070	3073	3076	rBV	284796	287850	1.84%	0.455%
23	21.104	3093	3097	3102	rBV	1466964	1830321	11.69%	2.891%
24	23.321	3468	3474	3482	rVB2	1035225	1896412	12.12%	2.996%

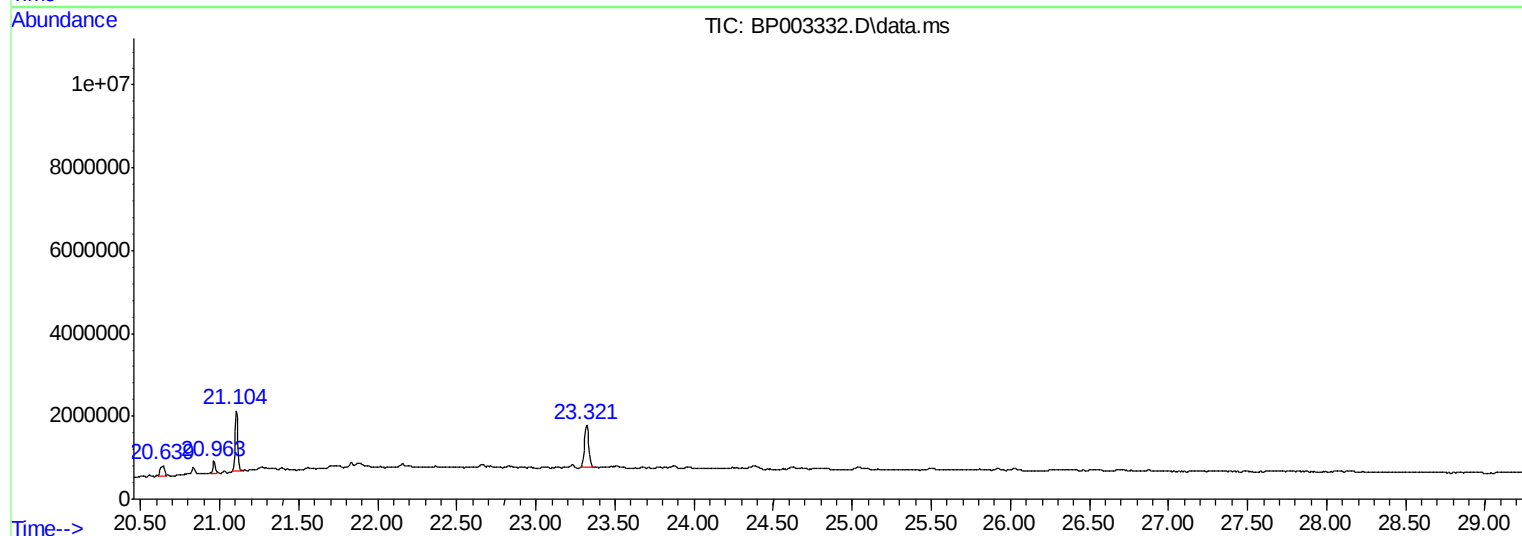
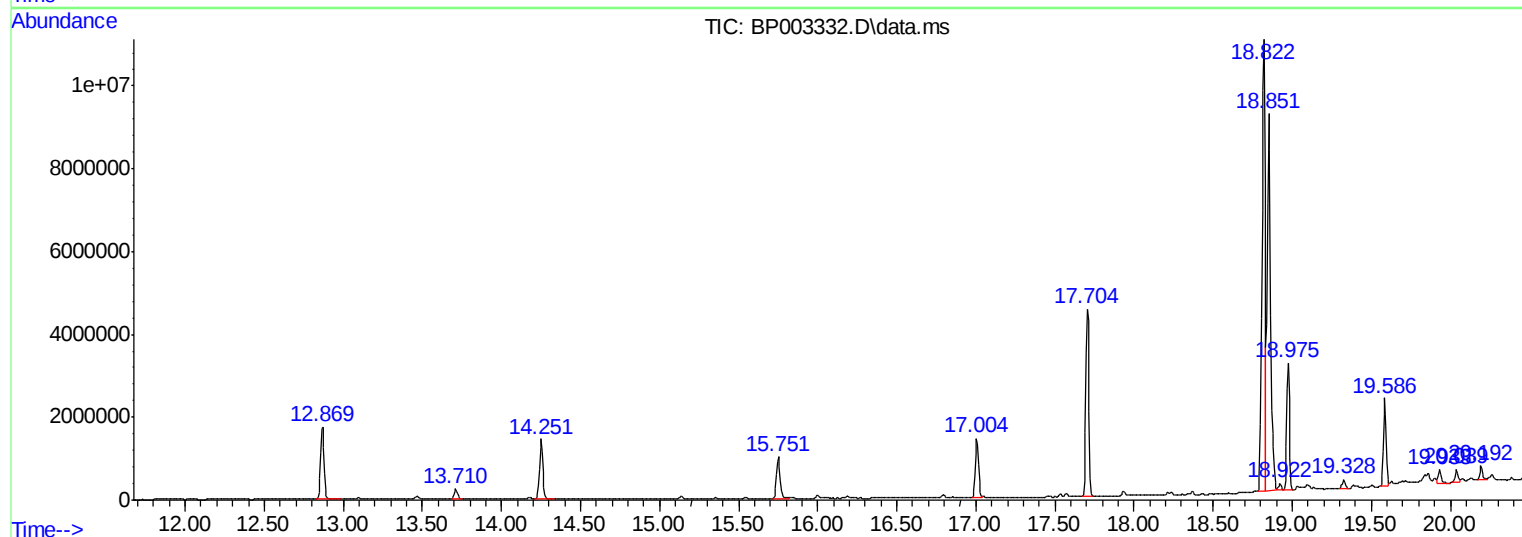
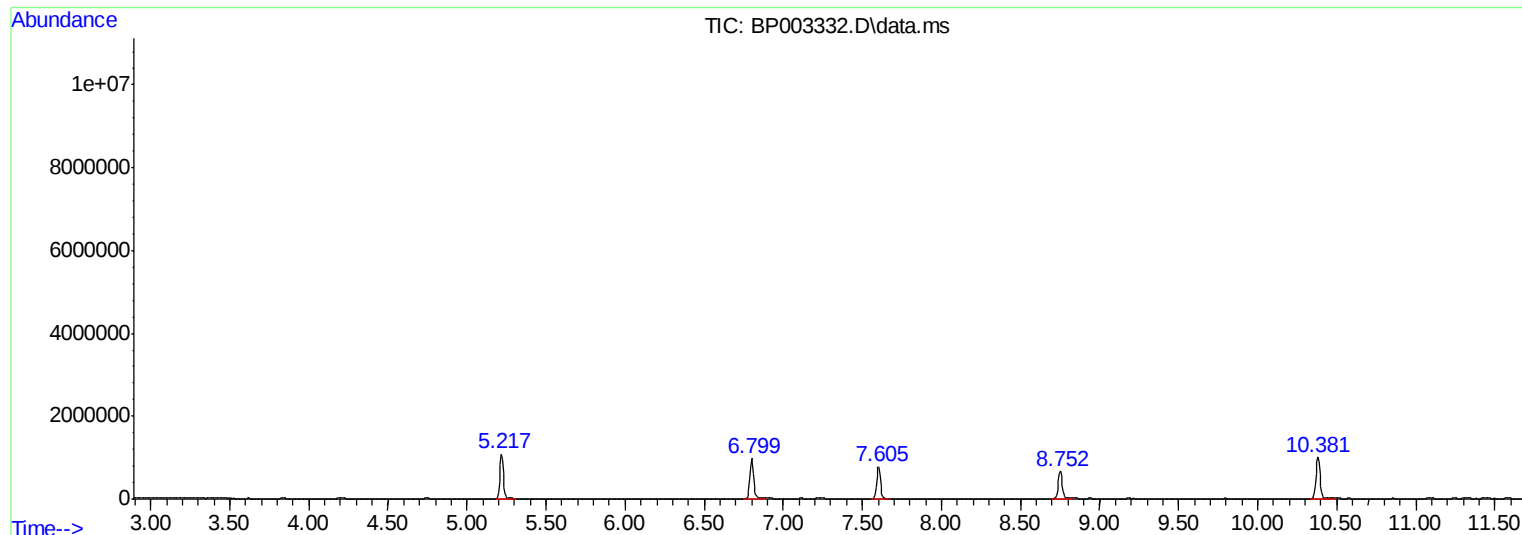
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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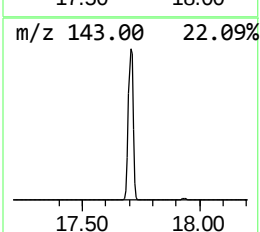
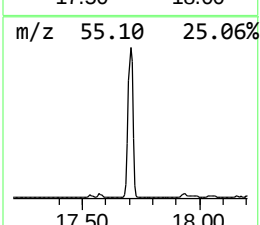
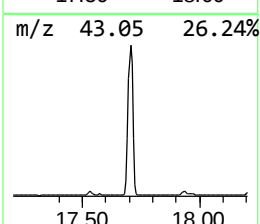
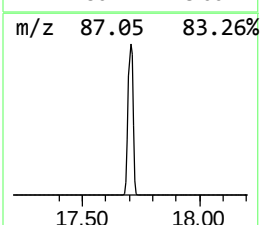
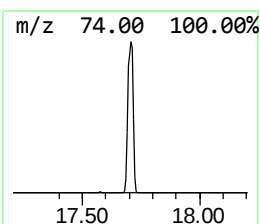
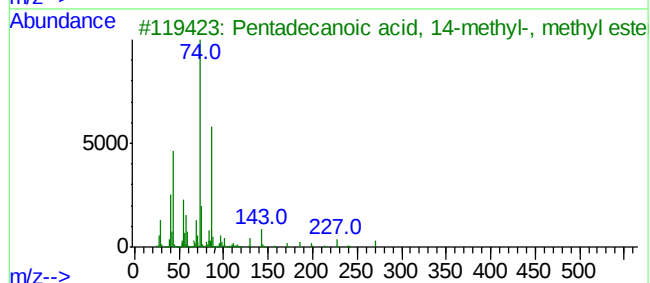
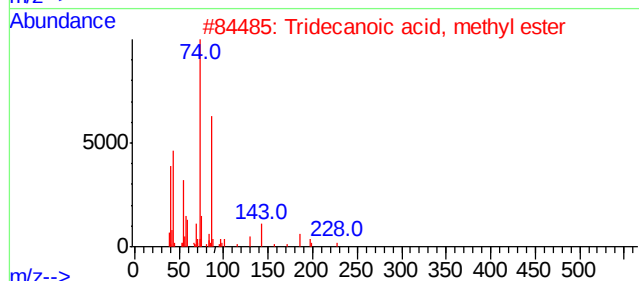
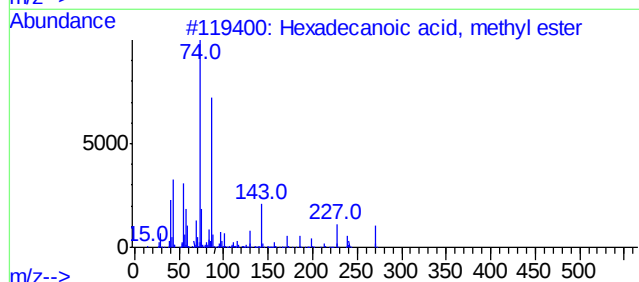
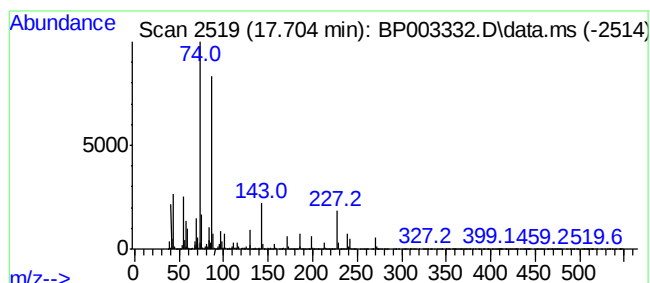
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.704	58.21 ng	5915260	Phenanthrene-d10	17.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	89
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
4	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	80
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	80



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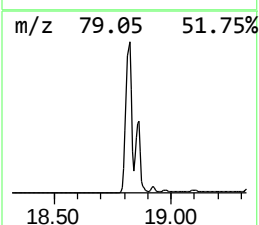
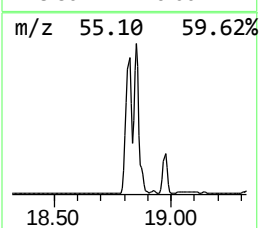
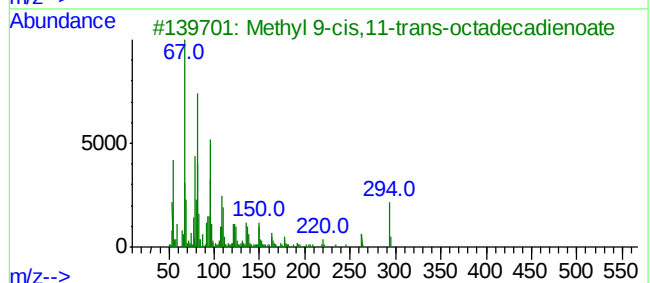
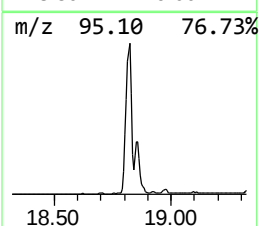
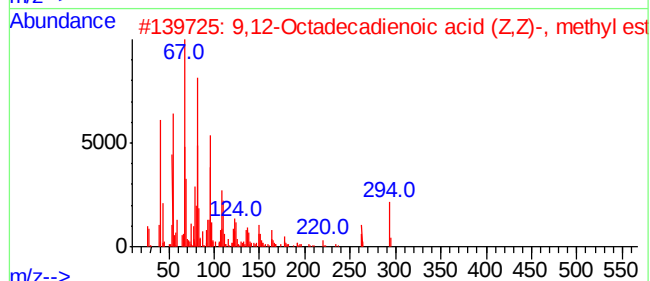
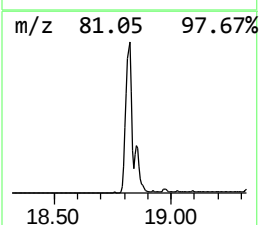
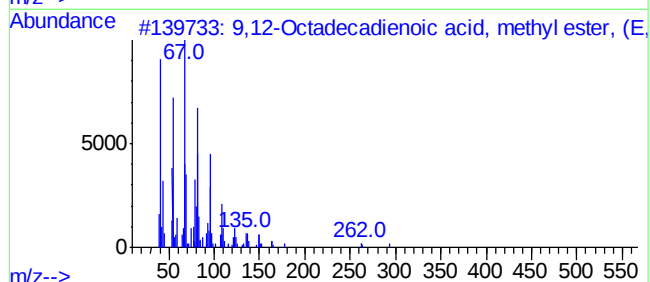
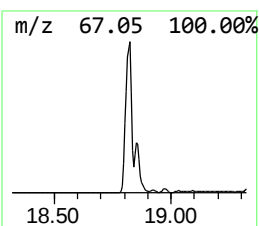
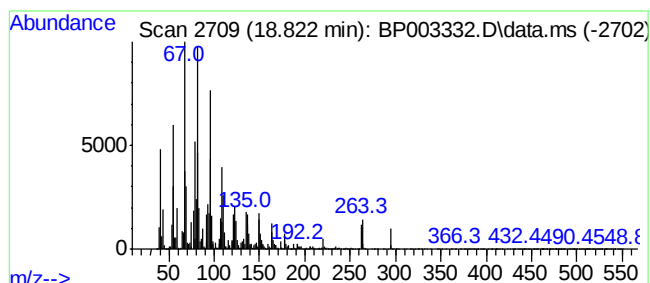
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.822	154.03 ng	15653100	Phenanthrene-d10	17.004

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99	
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99	
3	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99	
4	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99	
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99	



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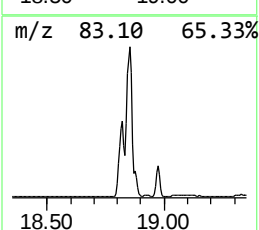
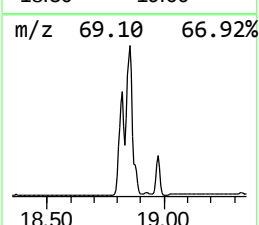
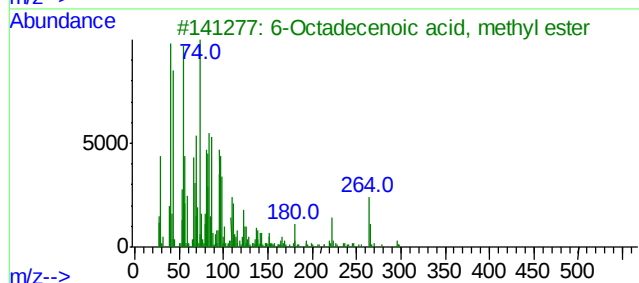
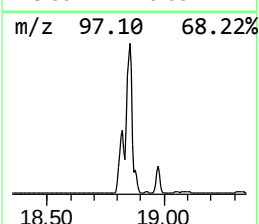
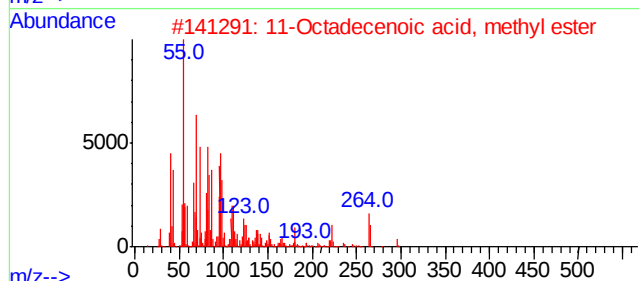
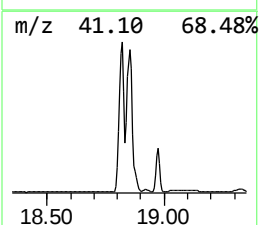
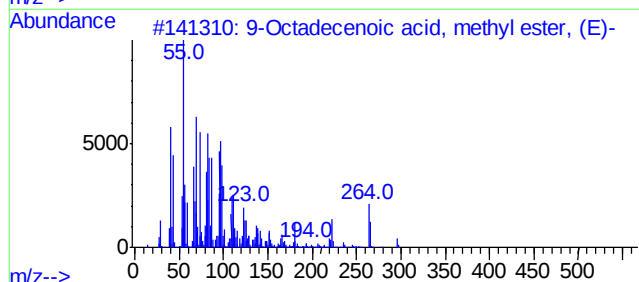
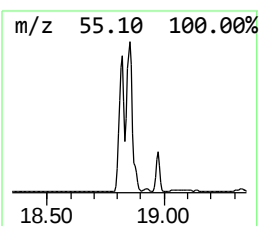
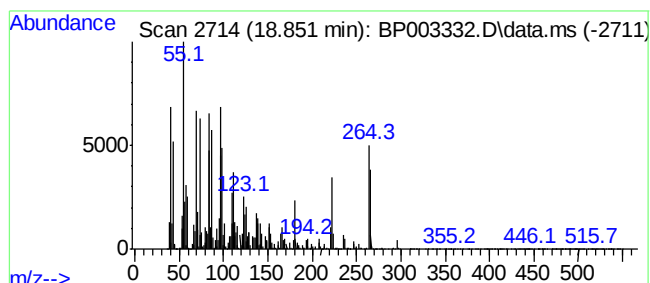
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.851	130.40 ng	13252000	Phenanthrene-d10	17.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	94
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	93
3	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	93
4	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	92
5	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	91



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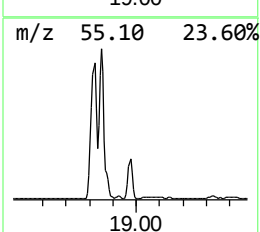
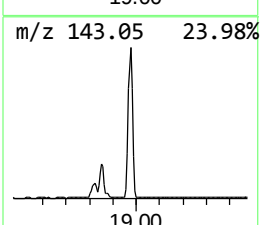
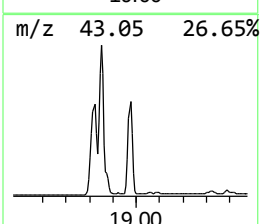
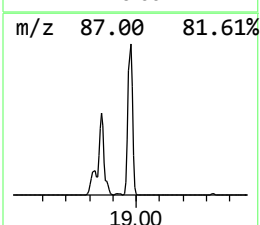
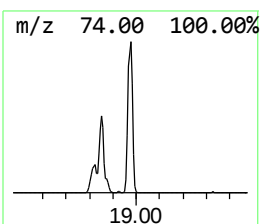
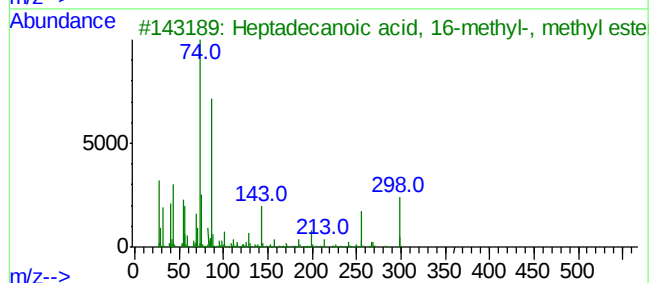
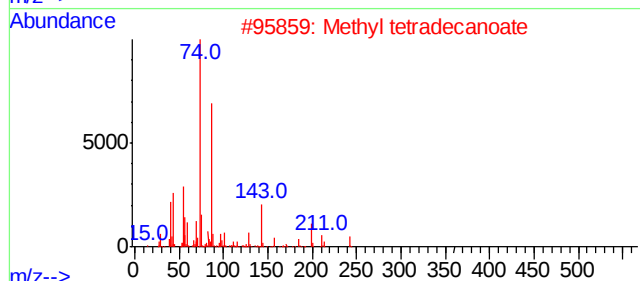
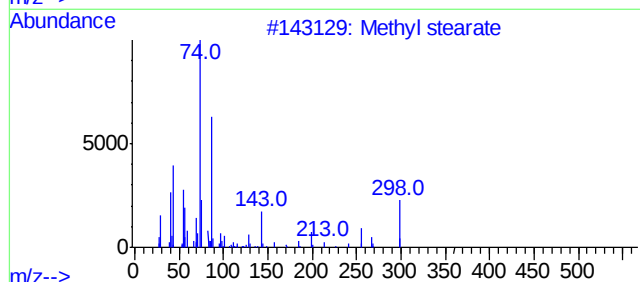
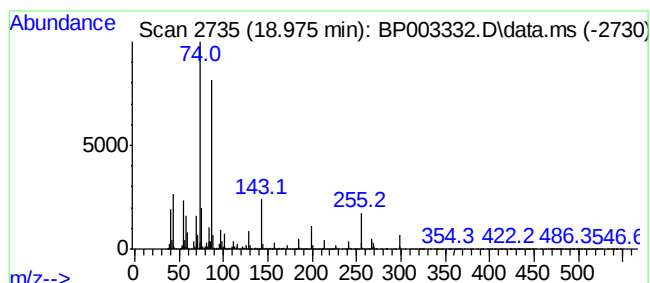
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Peak Number 4 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.975	34.78 ng	3534070	Phenanthrene-d10	17.004

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98	
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93	
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90	
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80	
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80	



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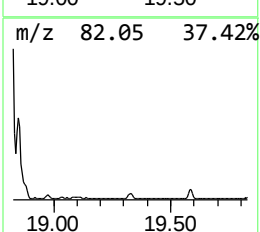
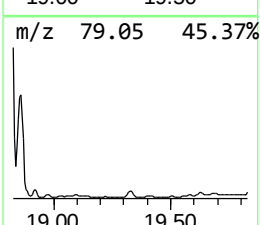
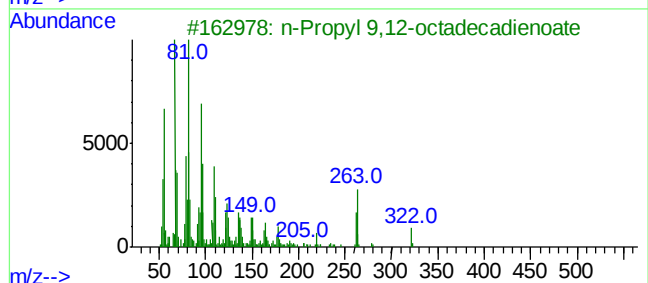
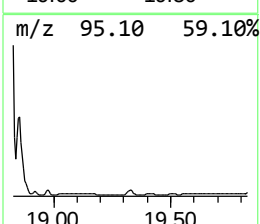
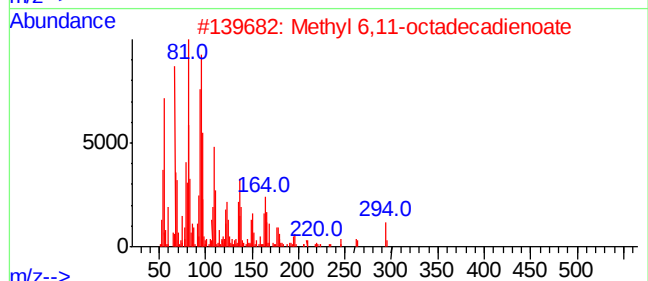
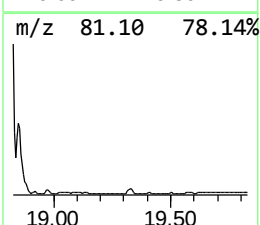
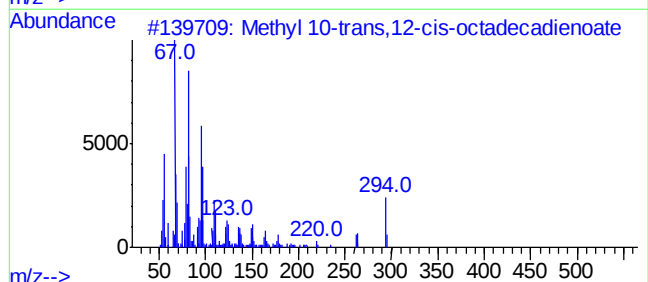
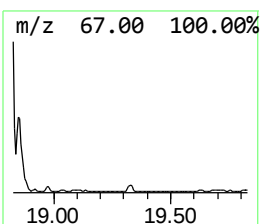
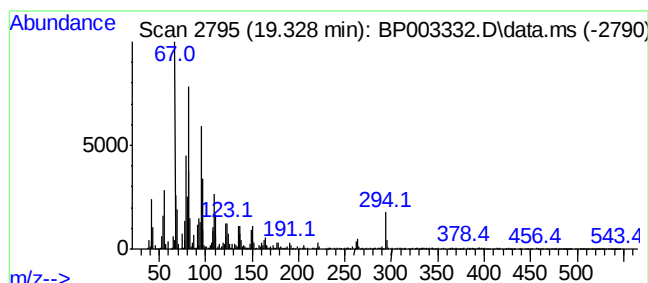
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Methyl 10-trans,12-cis-octa... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.328	3.34 ng	305222	Chrysene-d12	21.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98
2	Methyl 6,11-octadecadienoate	294	C19H34O2	1000336-43-2	93
3	n-Propyl 9,12-octadecadienoate	322	C21H38O2	1000336-77-8	91
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	89
5	7,10-Octadecadienoic acid, methy...	294	C19H34O2	056554-24-6	87



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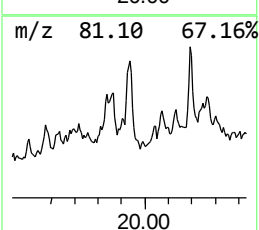
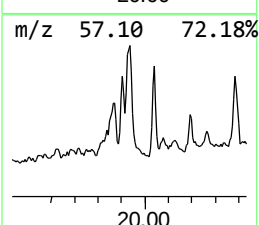
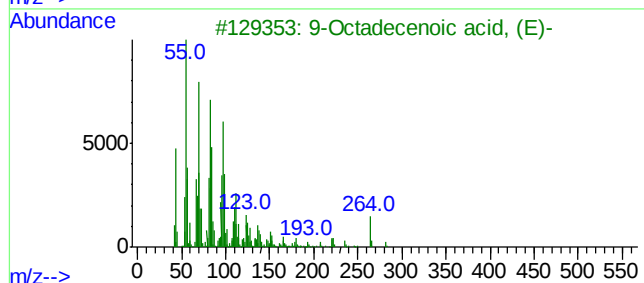
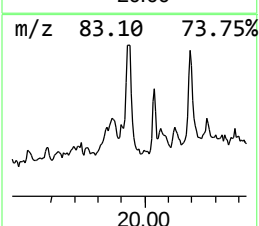
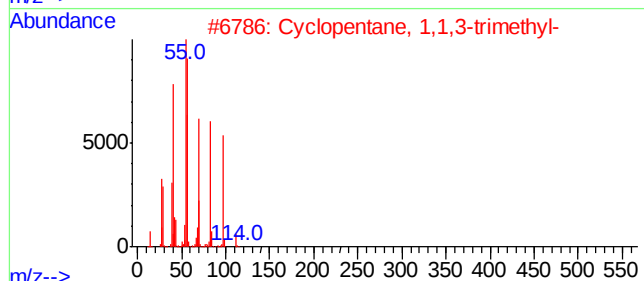
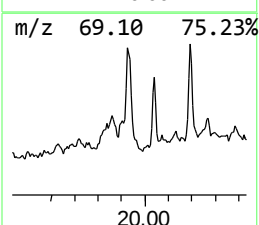
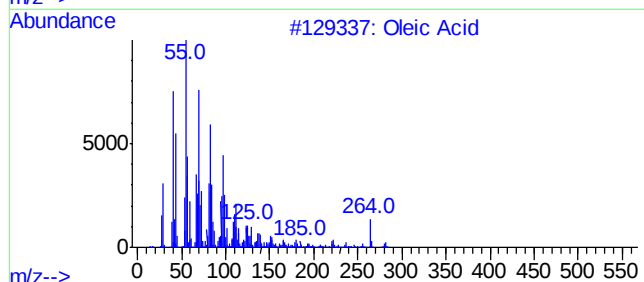
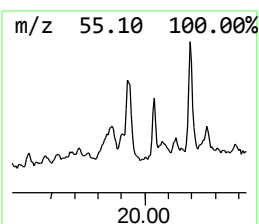
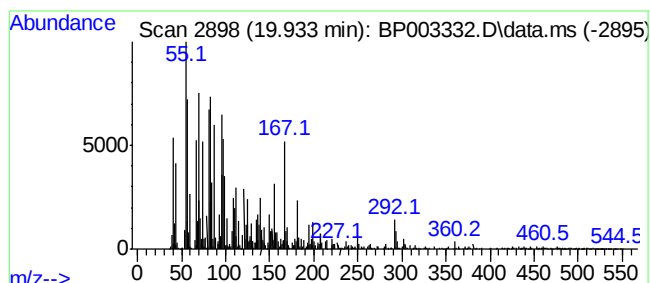
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BNA_P
ClientSampleId :
TR-05-091720

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Oleic Acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.933	4.87 ng	445337	Chrysene-d12		21.104	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Oleic Acid		282	C18H34O2	000112-80-1	90
2	Cyclopentane, 1,1,3-trimethyl-		112	C8H16	004516-69-2	50
3	9-Octadecenoic acid, (E)-		282	C18H34O2	000112-79-8	50
4	Cyclododecane		168	C12H24	000294-62-2	45
5	cis-13-Octadecenoic acid		282	C18H34O2	013126-39-1	44



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091820\
Data File : BP003332.D
Acq On : 18 Sep 2020 21:05
Operator : CG/JU
Sample : L3871-13 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-091720

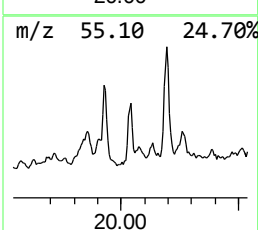
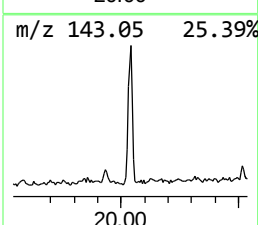
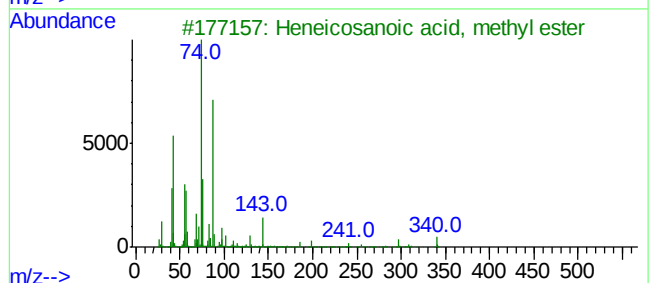
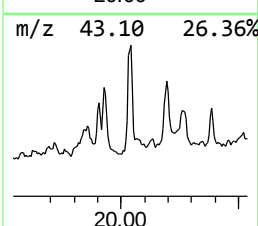
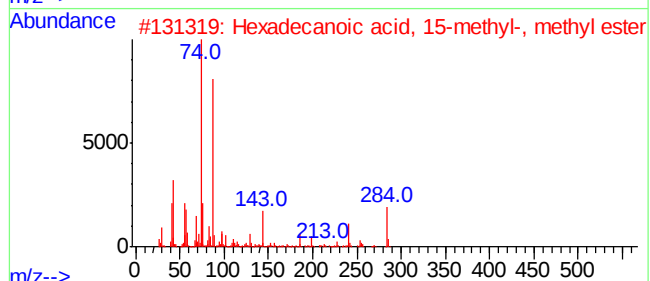
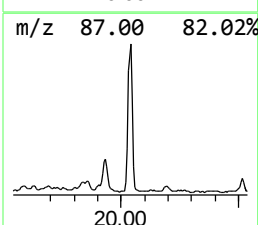
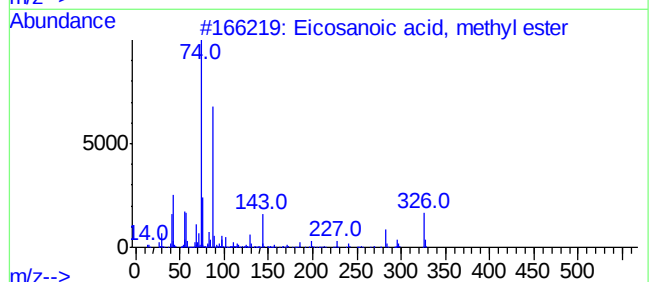
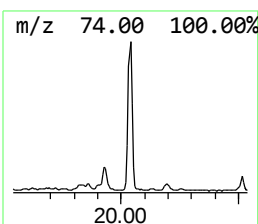
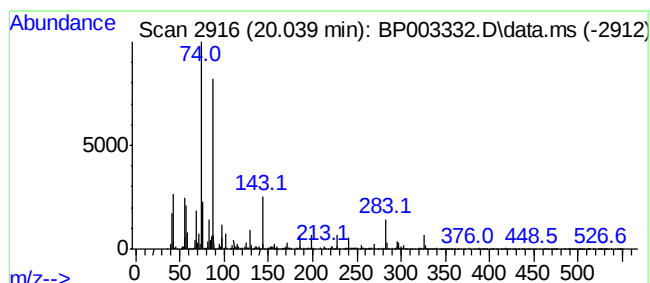
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Eicosanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.039	4.32 ng	394974	Chrysene-d12	21.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	98
2	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	96
3	Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	95
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091820\
Data File : BP003332.D
Acq On : 18 Sep 2020 21:05
Operator : CG/JU
Sample : L3871-13 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-091720

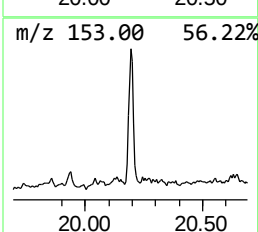
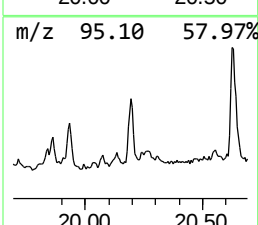
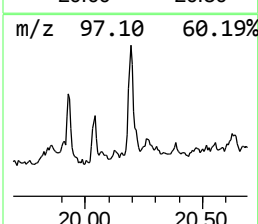
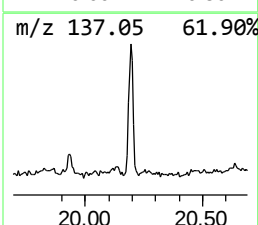
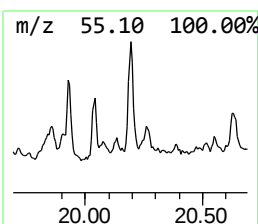
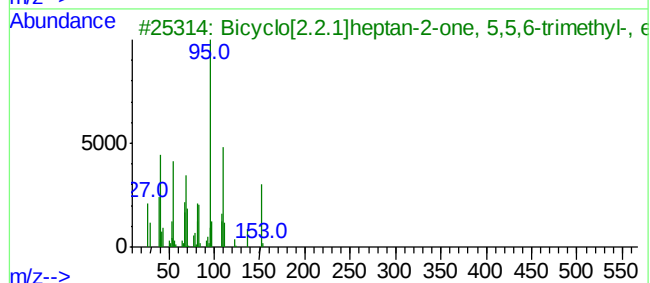
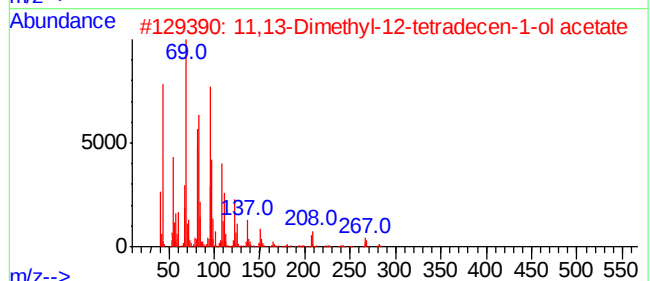
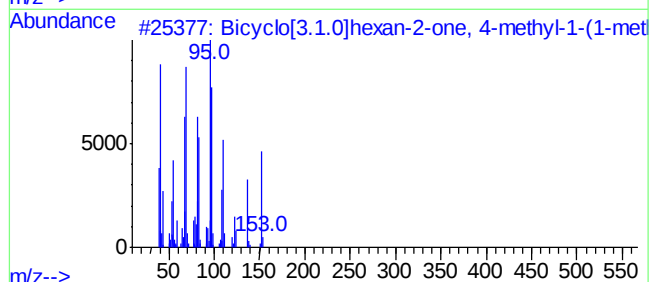
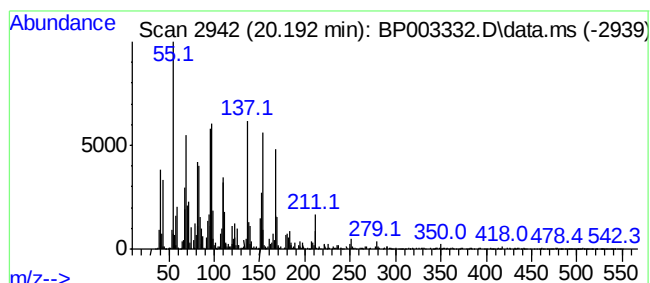
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown20.192 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.192	4.50 ng	411894	Chrysene-d12	21.104

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	46	
2	11,13-Dimethyl-12-tetradecen-1-o...	282	C18H34O2	1000130-81-0	30	
3	Bicyclo[2.2.1]heptan-2-one, 5,5,...	152	C10H16O	003649-86-3	22	
4	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	18	
5	(Z)-4-Methyl-5-(2-oxopropylidene...	152	C8H8O3	026474-45-3	18	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091820\
Data File : BP003332.D
Acq On : 18 Sep 2020 21:05
Operator : CG/JU
Sample : L3871-13 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-091720

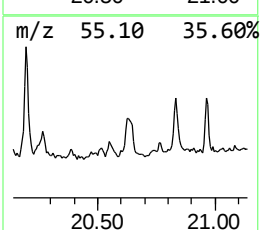
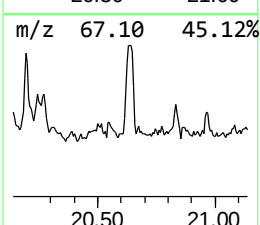
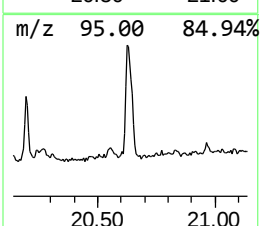
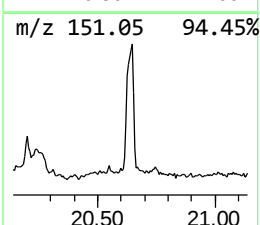
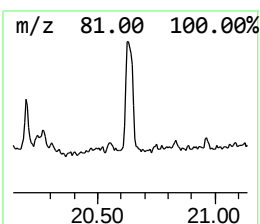
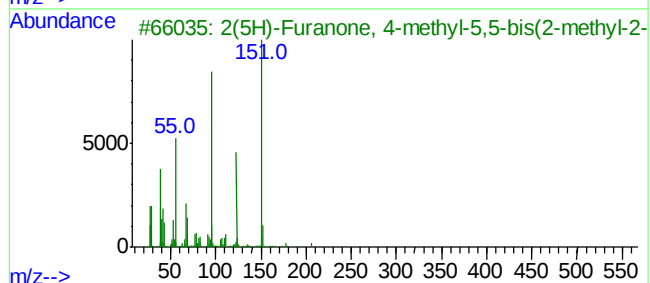
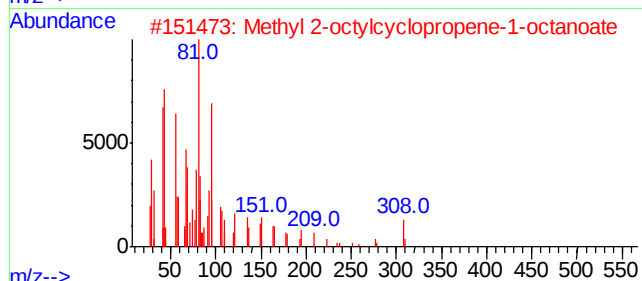
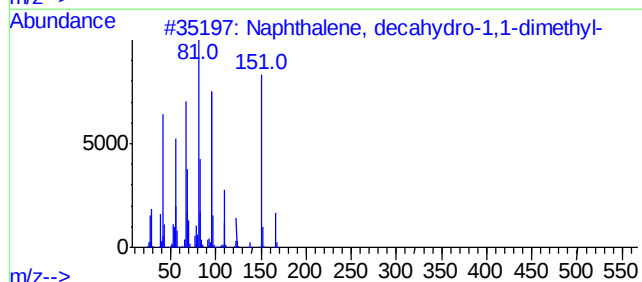
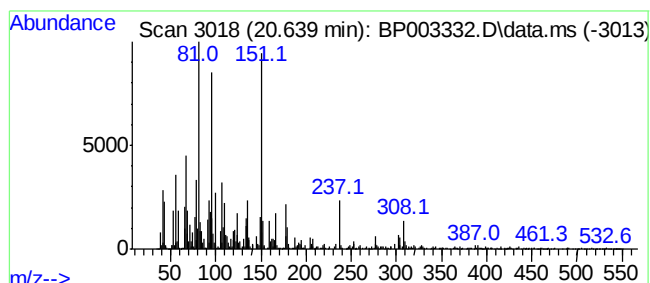
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown20.639 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.639	4.84 ng	442684	Chrysene-d12	21.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-1,1-dimet...	166	C12H22	035431-04-0	46
2	Methyl 2-octylcyclopropene-1-oct...	308	C20H36O2	003220-60-8	38
3	2(5H)-Furanone, 4-methyl-5,5-bis...	206	C13H18O2	099202-98-9	30
4	Bicyclo[2.2.1]heptane, 2-(2-meth...	150	C11H18	061142-27-6	27
5	2,3-Bornanediol	170	C10H18O2	025696-56-4	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091820\
Data File : BP003332.D
Acq On : 18 Sep 2020 21:05
Operator : CG/JU
Sample : L3871-13 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-05-091720

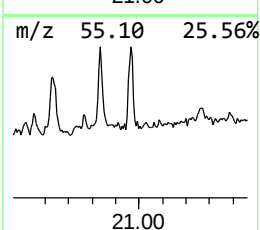
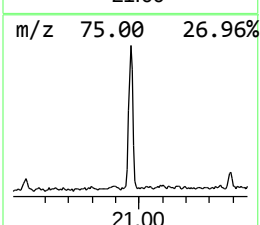
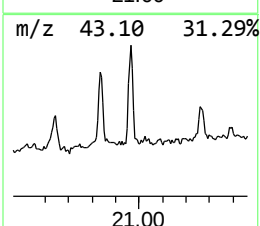
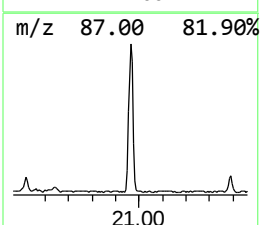
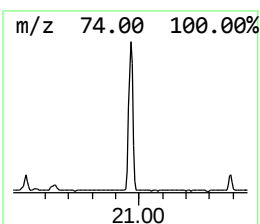
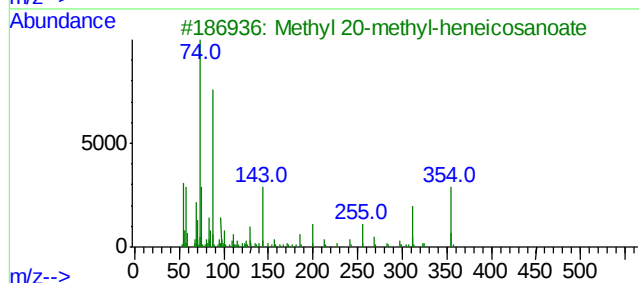
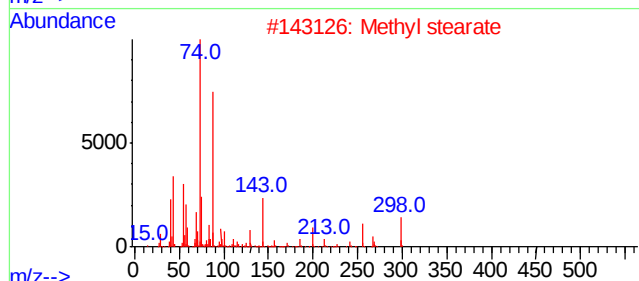
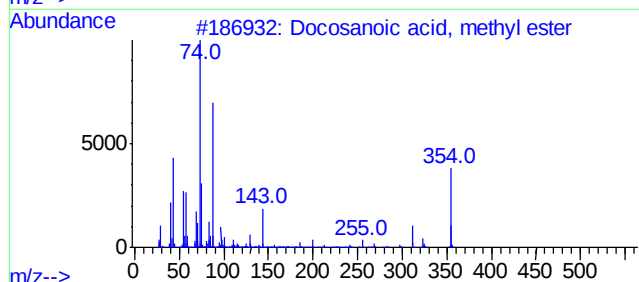
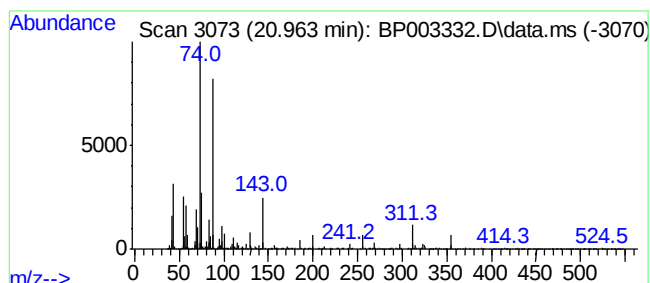
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Docosanoic acid, methyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.963	3.15 ng	287850	Chrysene-d12	21.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	99
2	Methyl stearate	298	C19H38O2	000112-61-8	97
3	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	95
4	Octacosanoic acid, methyl ester	438	C29H58O2	055682-92-3	87
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091820\
 Data File : BP003332.D
 Acq On : 18 Sep 2020 21:05
 Operator : CG/JU
 Sample : L3871-13 2X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TR-05-091720

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecanoic ac...	17.704	58.2	ng	5915260	4	17.004	2032470	20.0
9,12-Octadecadi...	18.822	154.0	ng	15653100	4	17.004	2032470	20.0
9-Octadecenoic ...	18.851	130.4	ng	13252000	4	17.004	2032470	20.0
Methyl stearate	18.975	34.8	ng	3534070	4	17.004	2032470	20.0
Methyl 10-trans...	19.328	3.3	ng	305222	5	21.104	1830320	20.0
Oleic Acid	19.933	4.9	ng	445337	5	21.104	1830320	20.0
Eicosanoic acid...	20.039	4.3	ng	394974	5	21.104	1830320	20.0
unknown20.192	20.192	4.5	ng	411894	5	21.104	1830320	20.0
unknown20.639	20.639	4.8	ng	442684	5	21.104	1830320	20.0
Docosanoic acid...	20.963	3.1	ng	287850	5	21.104	1830320	20.0