

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
 Data File : BF130382.D
 Acq On : 22 Sep 2022 18:43
 Operator : CG\JU
 Sample : N4752-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-07-092122

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130382.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.257	535	539	543	rBV	2047000	1984231	13.36%	4.017%
2	6.299	711	716	733	rBV	1991422	1948283	13.12%	3.944%
3	6.651	773	776	780	rBV	804402	715863	4.82%	1.449%
4	7.222	868	873	876	rBV	1416529	1227627	8.27%	2.485%
5	7.934	990	994	998	rBV	963564	887373	5.98%	1.797%
6	9.016	1173	1178	1181	rBV	2352120	1999088	13.46%	4.047%
7	9.687	1285	1292	1295	rBV	1046619	823080	5.54%	1.666%
8	10.475	1422	1426	1429	rBV	1165536	1028994	6.93%	2.083%
9	11.169	1540	1544	1546	rBV	836040	682148	4.59%	1.381%
10	11.575	1609	1613	1616	rBV	3963829	3348563	22.55%	6.779%
11	11.716	1631	1637	1644	rBV2	863520	1010376	6.80%	2.046%
12	12.275	1725	1732	1734	rBV	9627160	14848087	100.00%	30.061%
13	12.298	1734	1736	1741	rVB2	9775350	8385794	56.48%	16.978%
14	12.369	1745	1748	1751	rBV2	2672816	2289959	15.42%	4.636%
15	12.416	1751	1756	1758	rBV	1886382	2608420	17.57%	5.281%
16	12.498	1768	1770	1774	rVB	176223	149219	1.00%	0.302%
17	12.604	1783	1788	1791	rBV	392422	403804	2.72%	0.818%
18	12.757	1810	1814	1817	rBV	1936626	1624036	10.94%	3.288%
19	12.963	1842	1849	1852	rVB3	188374	336295	2.26%	0.681%
20	13.010	1852	1857	1859	rBV3	146964	193847	1.31%	0.392%
21	13.086	1867	1870	1874	rBV	215119	211897	1.43%	0.429%
22	13.516	1940	1943	1946	rVB2	161120	190204	1.28%	0.385%
23	13.757	1981	1984	1987	rBV	245036	197232	1.33%	0.399%
24	13.798	1987	1991	1994	rBV2	719528	811786	5.47%	1.644%
25	13.904	2004	2009	2012	rBV	258016	277905	1.87%	0.563%
26	14.804	2159	2162	2169	rVB	151327	253642	1.71%	0.514%
27	15.198	2225	2229	2232	rBV	374636	444455	2.99%	0.900%
28	15.833	2334	2337	2347	rVB2	130841	265386	1.79%	0.537%
29	16.221	2400	2403	2413	rVB	132467	245568	1.65%	0.497%

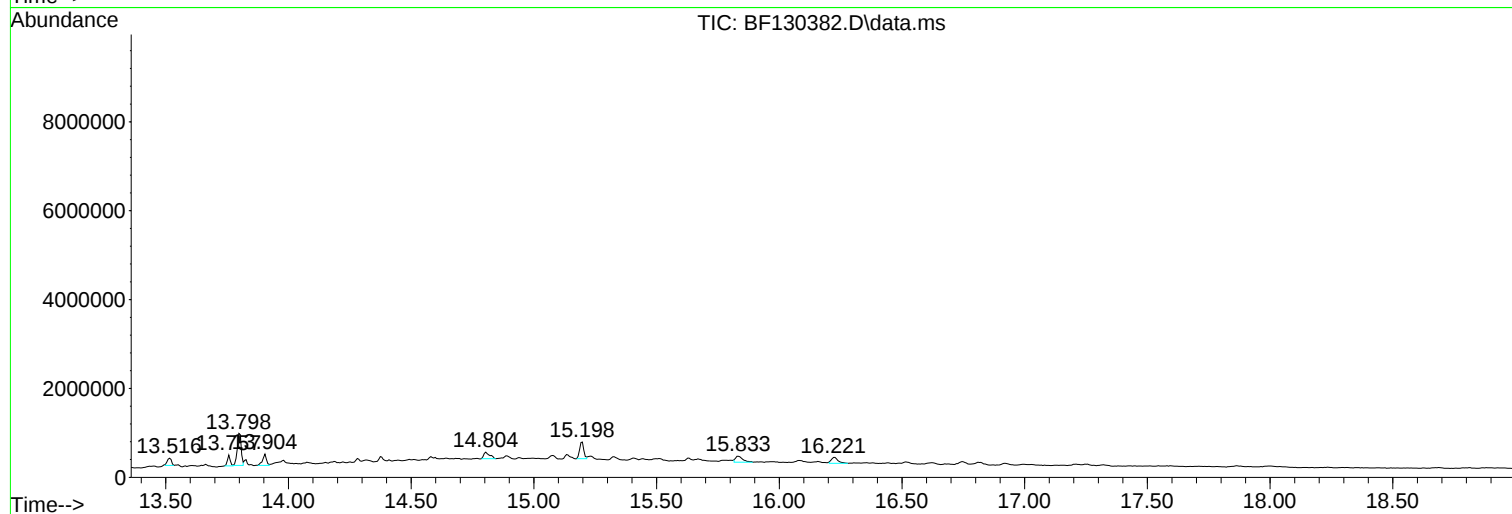
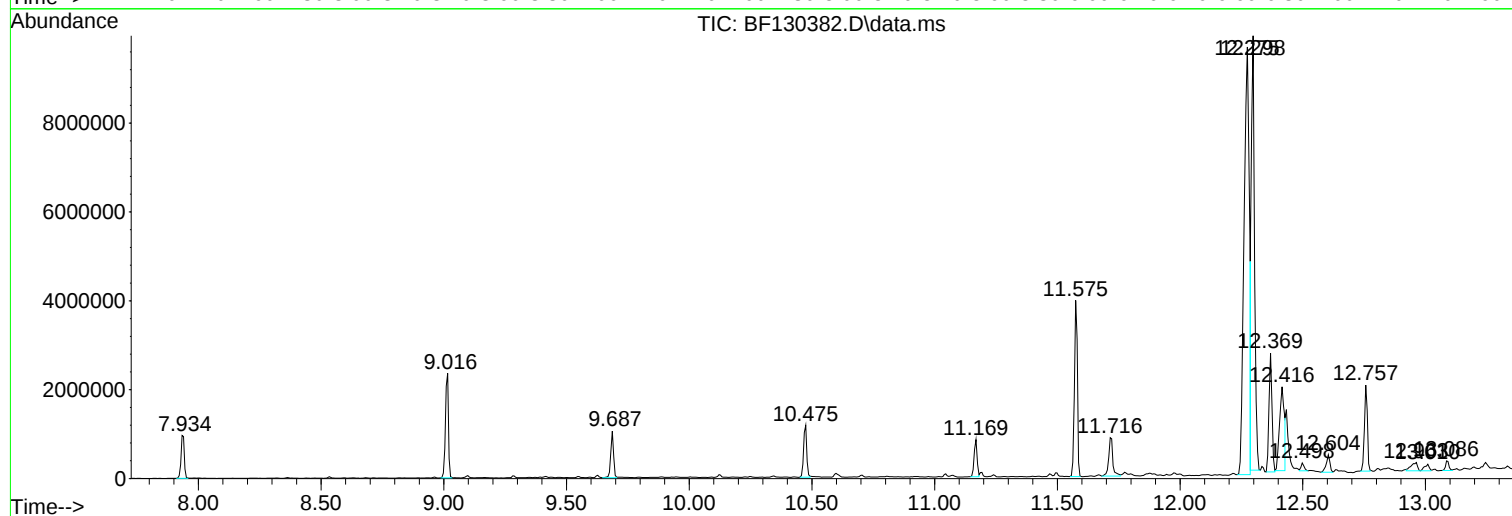
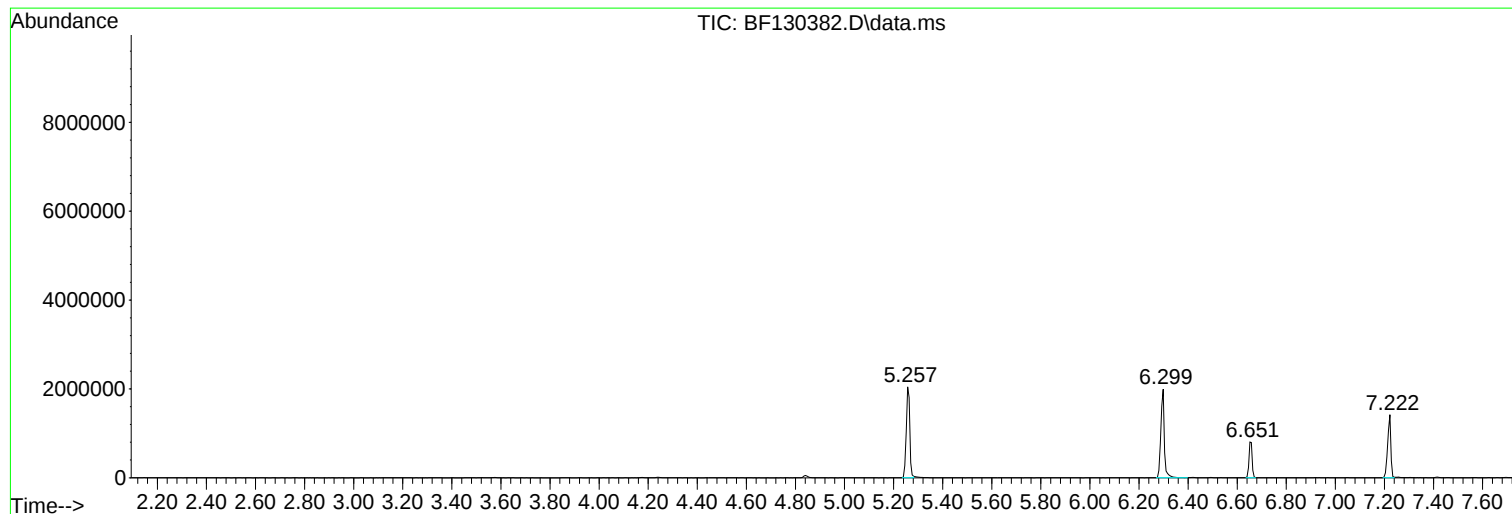
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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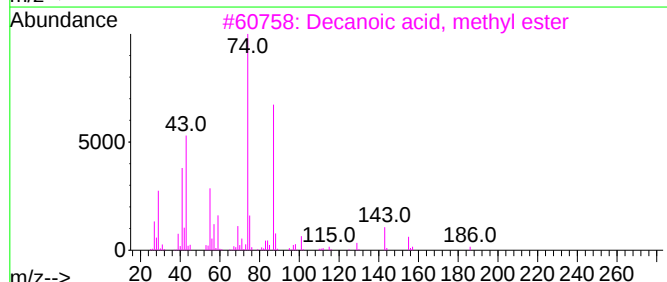
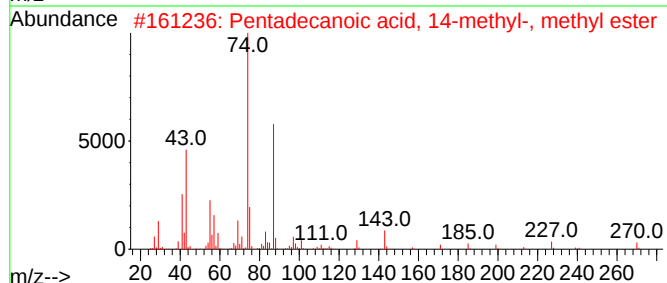
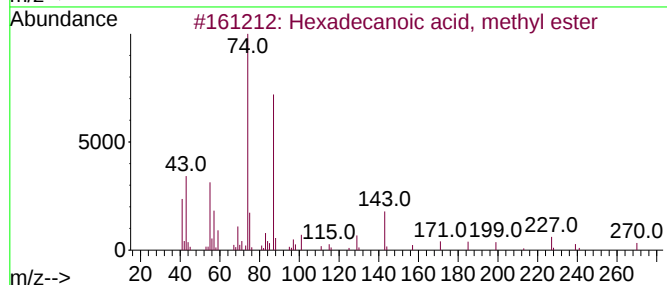
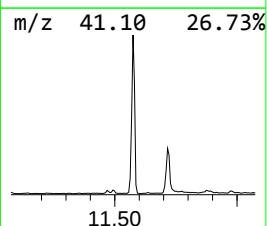
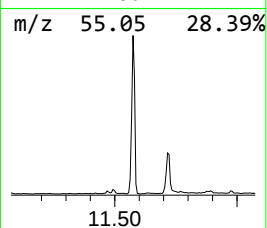
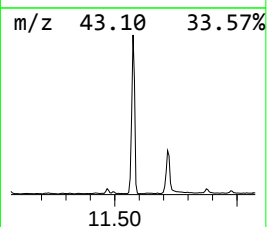
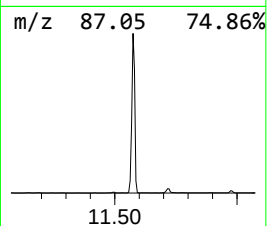
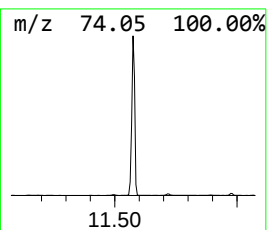
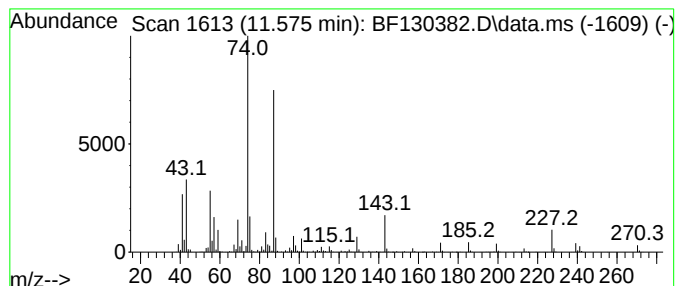
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.575	98.18 ng	3348560	Phenanthrene-d10		11.169	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...		270	C17H34O2	005129-60-2	93
3	Decanoic acid, methyl ester		186	C11H22O2	000110-42-9	87
4	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	86
5	Tridecanoic acid, 12-methyl-, me...		242	C15H30O2	005129-58-8	83



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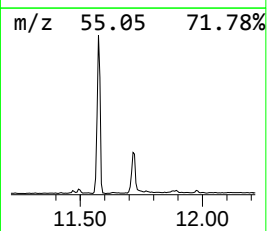
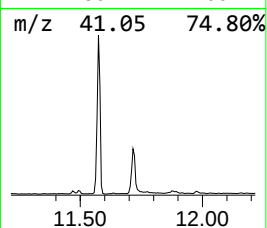
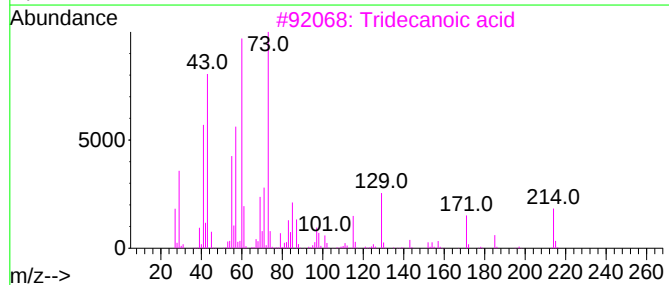
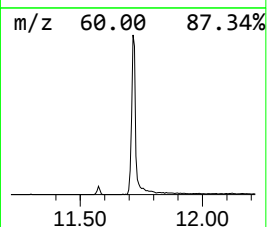
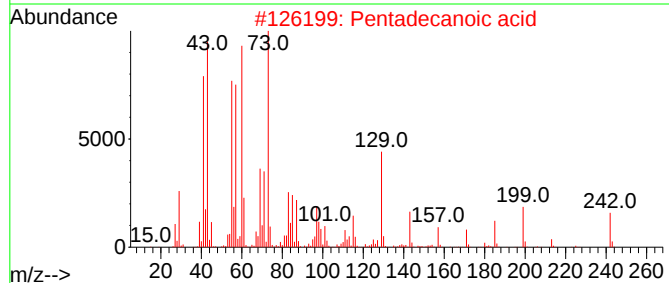
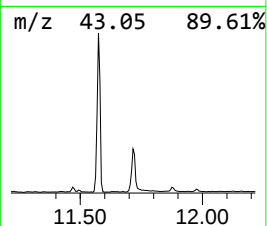
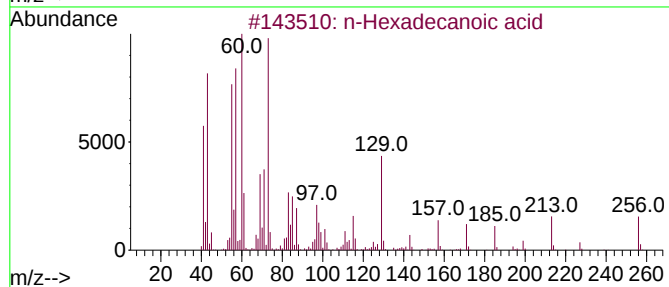
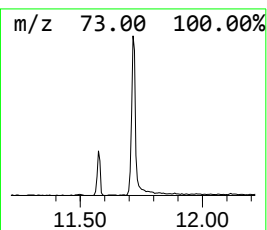
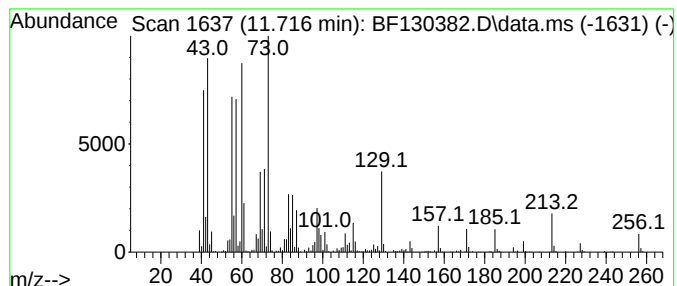
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.716	29.62 ng	1010380	Phenanthrene-d10	11.169

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	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	35



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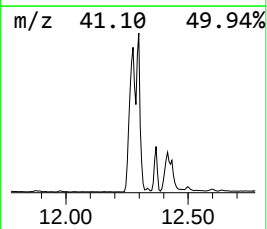
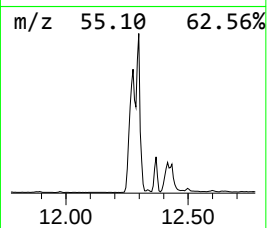
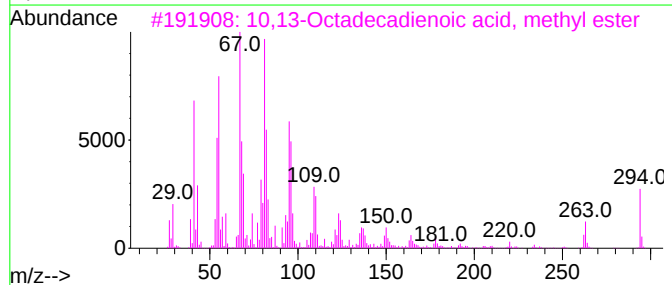
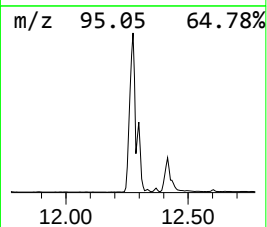
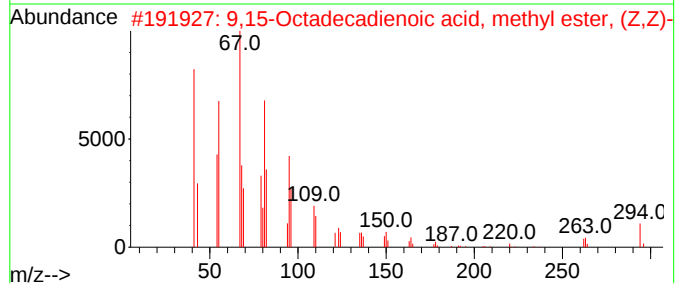
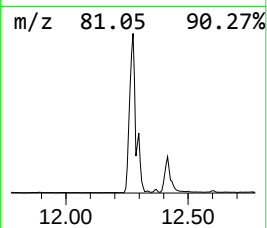
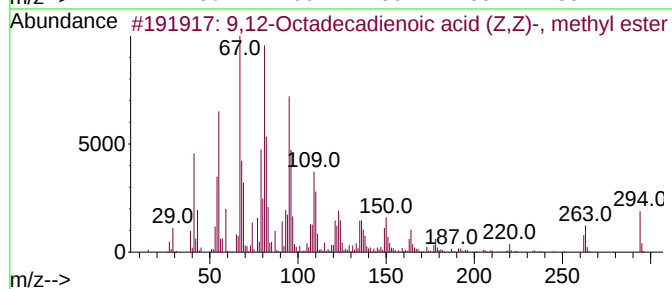
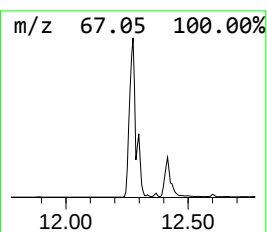
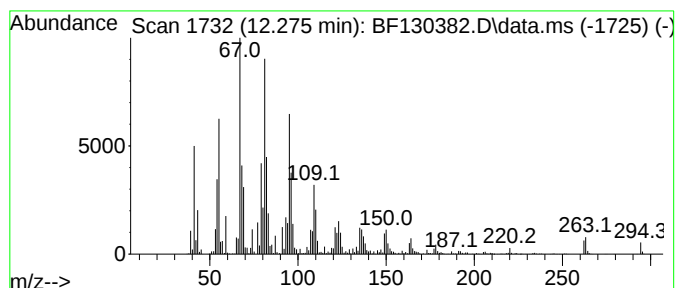
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.275	435.33 ng	14848100	Phenanthrene-d10	11.169	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99



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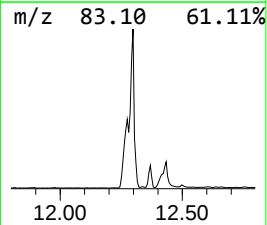
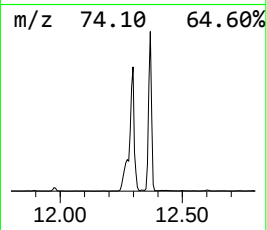
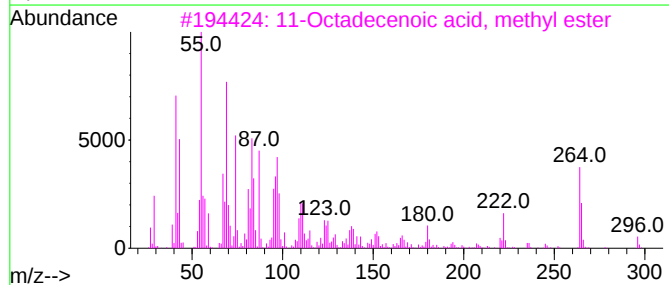
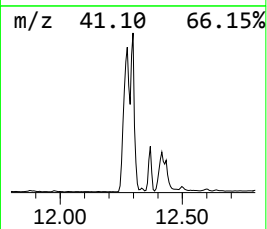
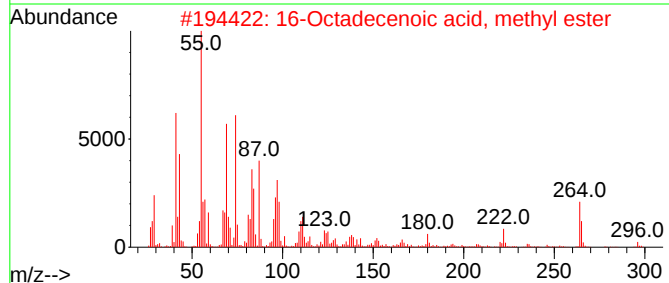
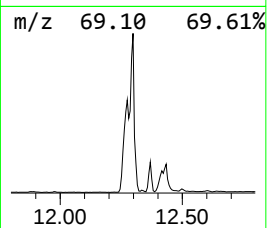
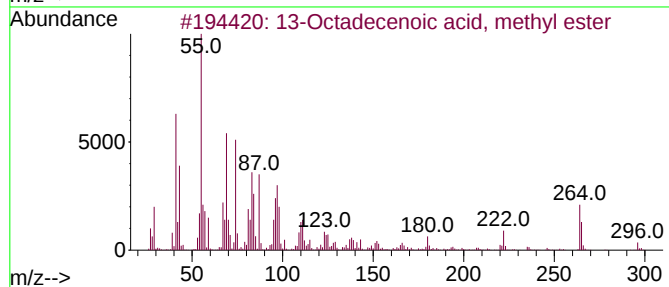
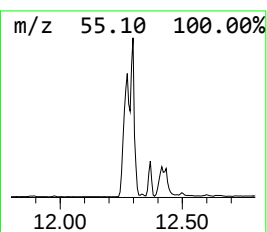
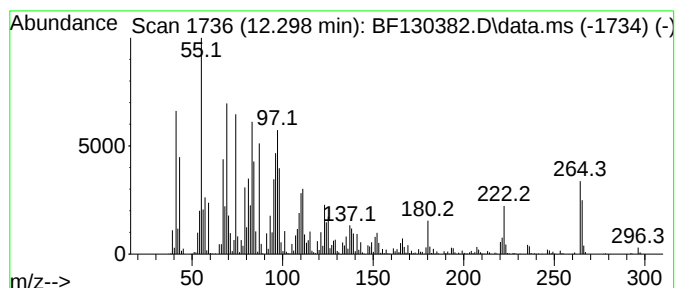
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Peak Number 4 13-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.298	245.86 ng	8385790	Phenanthrene-d10	11.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
2			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
3			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
4			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
5			6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	98



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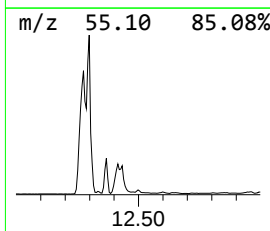
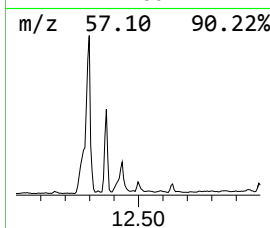
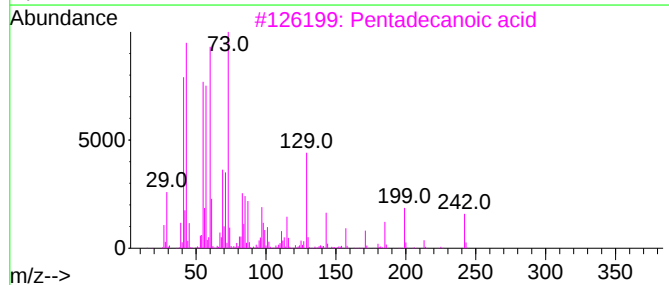
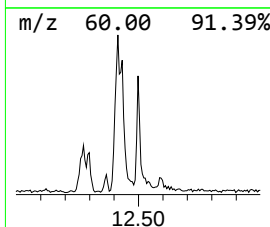
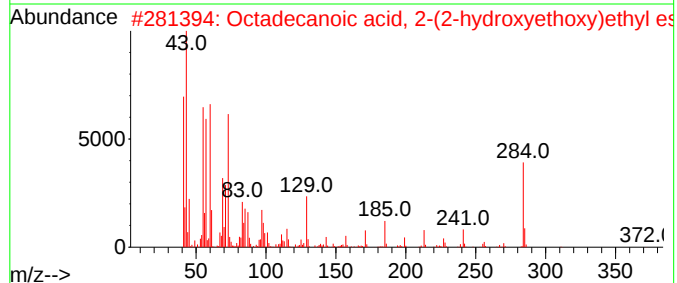
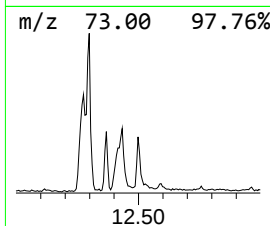
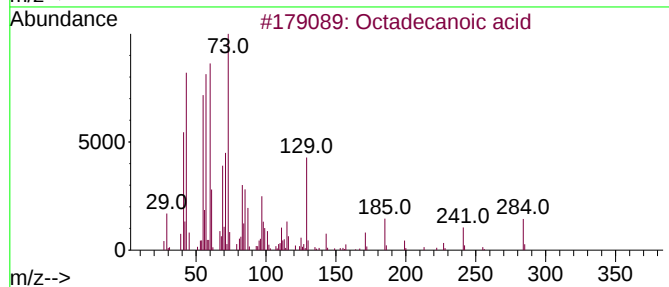
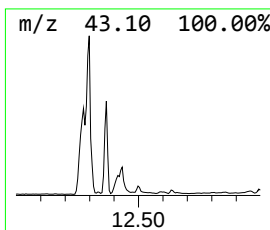
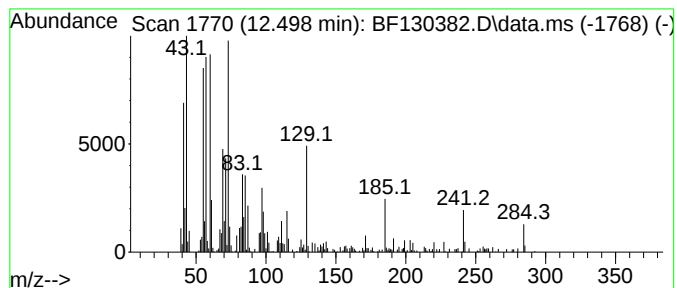
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Peak Number 5 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	3.68 ng	149219	Chrysene-d12	13.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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ALS Vial : 11 Sample Multiplier: 1

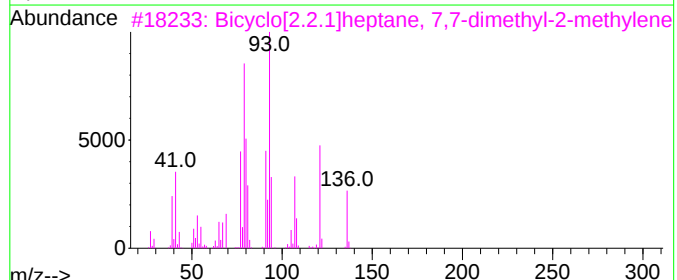
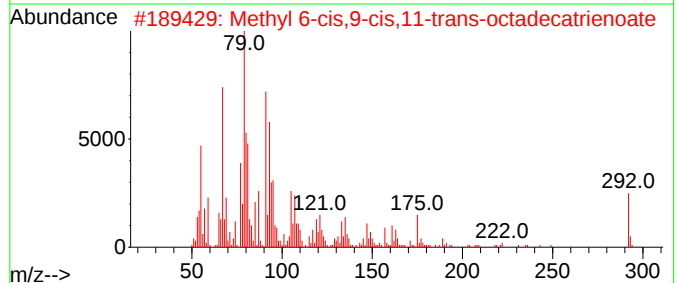
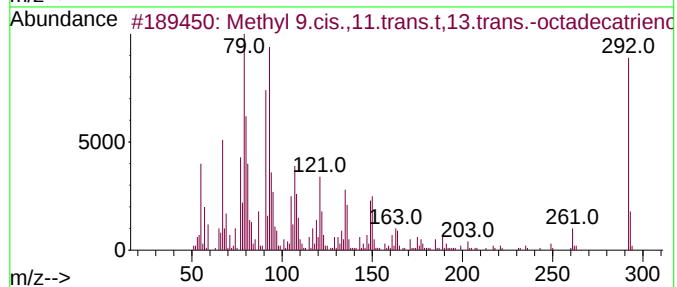
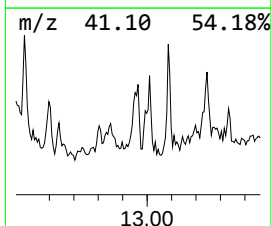
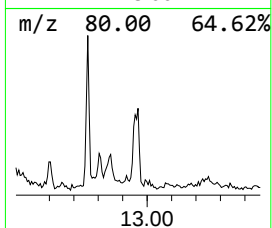
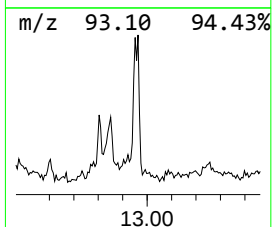
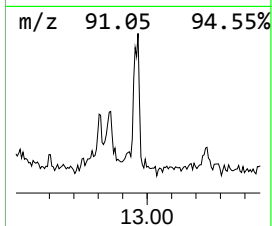
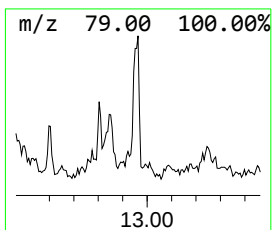
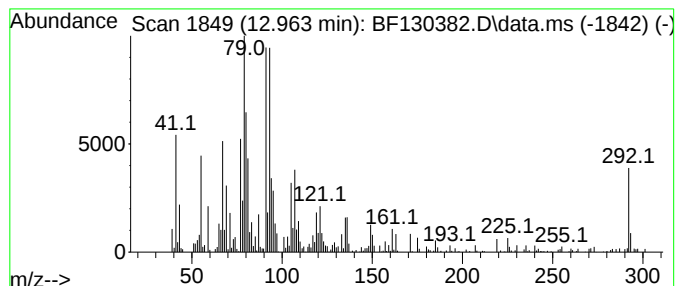
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ClientSampleId :
NB-07-092122

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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 Methyl 9.cis.,11.trans.t,13... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.963	8.29 ng	336295	Chrysene-d12	13.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9.cis.,11.trans.t,13.tran...	292	C19H32O2	1000336-42-6	94
2	Methyl 6-cis,9-cis,11-trans-octa...	292	C19H32O2	1010336-37-7	72
3	Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	70
4	cis-3-Butyl-4-vinyl-cyclopentene	150	C11H18	093779-52-3	70
5	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	016022-04-1	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130382.D
Acq On : 22 Sep 2022 18:43
Operator : CG\JU
Sample : N4752-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

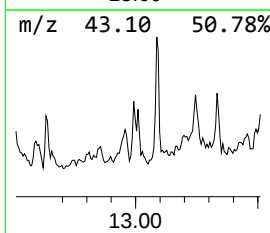
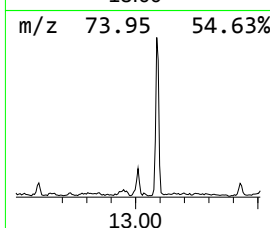
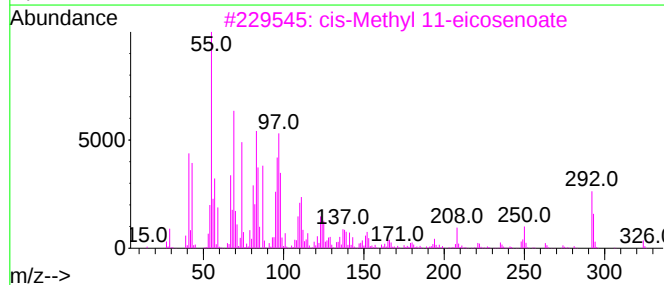
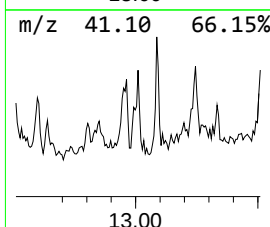
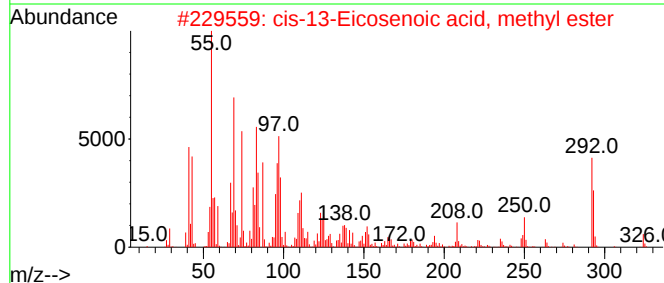
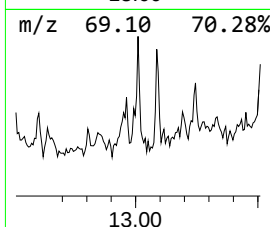
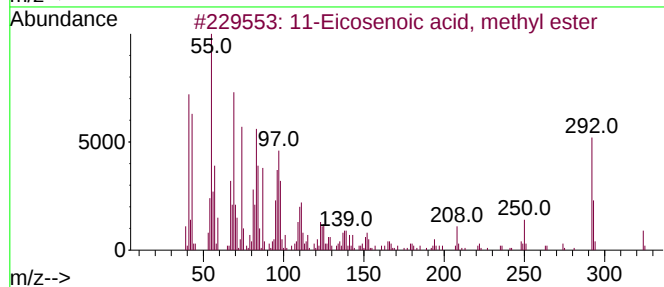
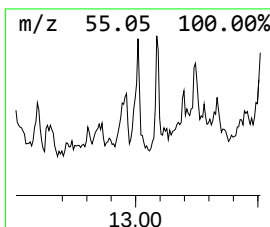
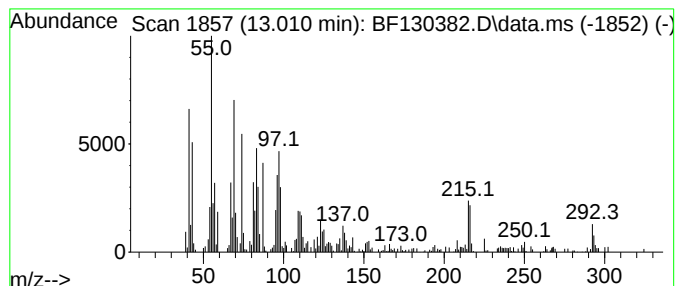
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11-Eicosenoic acid, methyl ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.010	4.78 ng	193847	Chrysene-d12	13.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	99
2	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	99
3	cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	99
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
5	Methyl (Z)-10-pentadecenoate	254	C16H30O2	1000426-92-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130382.D
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Operator : CG\JU
Sample : N4752-01
Misc :
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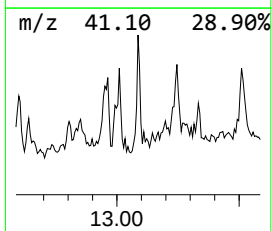
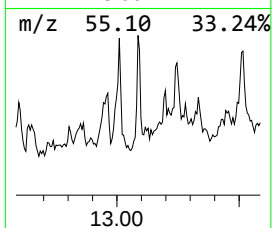
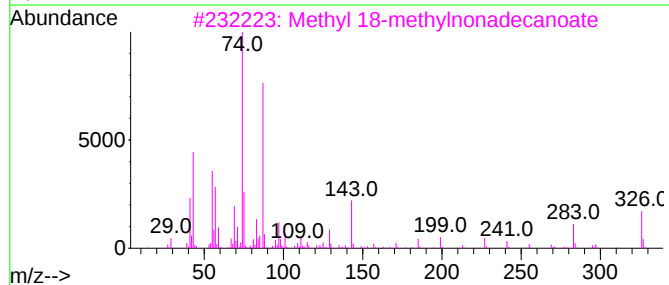
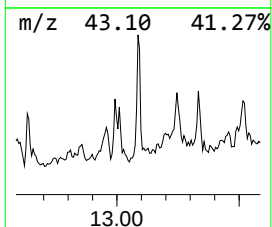
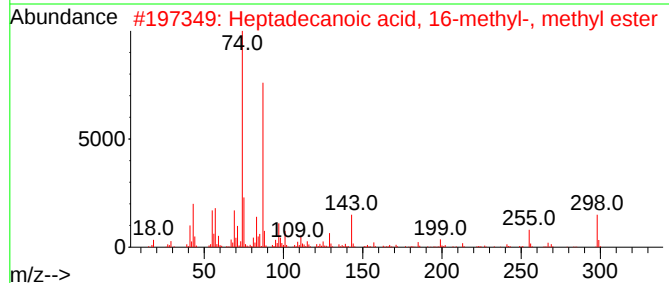
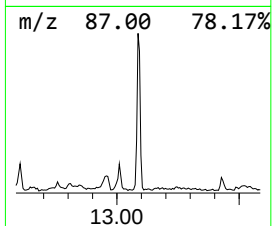
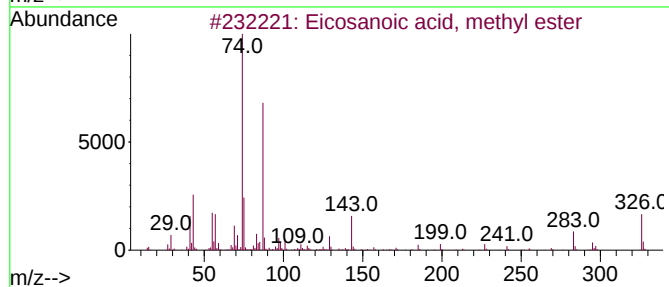
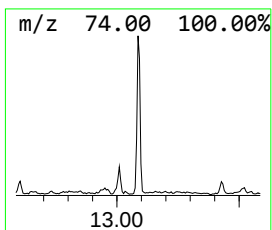
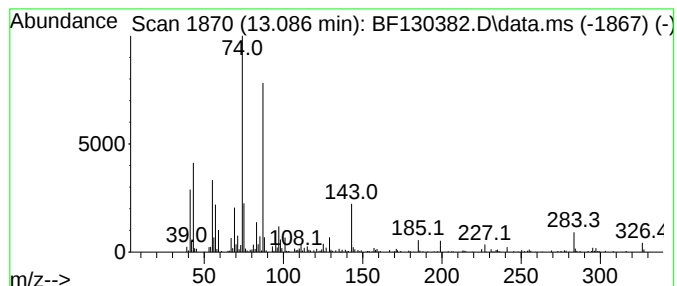
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.086	5.22 ng	211897	Chrysene-d12	13.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
3	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	91
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130382.D
Acq On : 22 Sep 2022 18:43
Operator : CG\JU
Sample : N4752-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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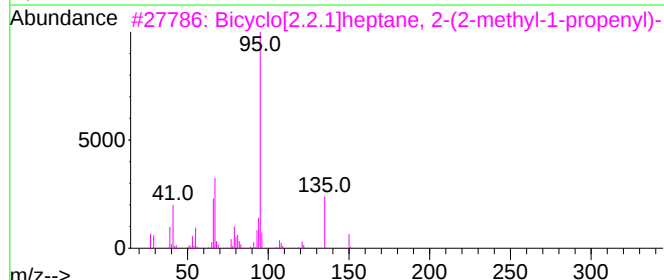
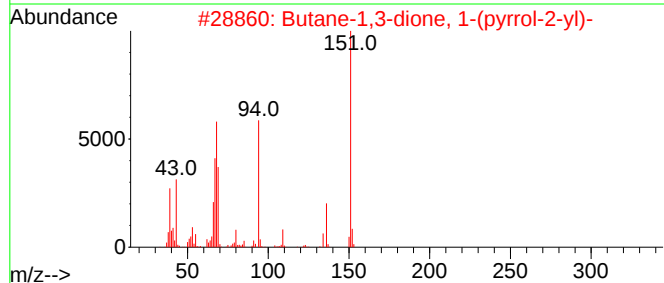
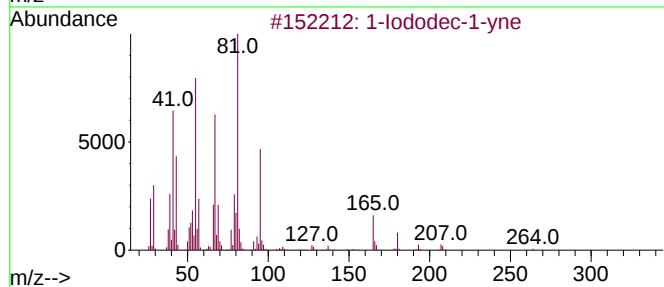
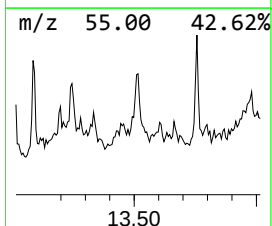
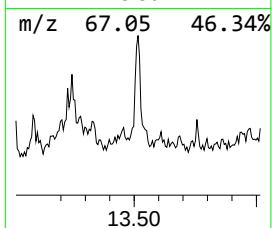
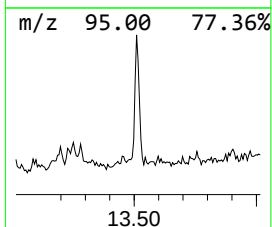
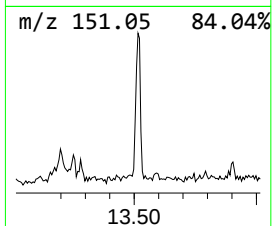
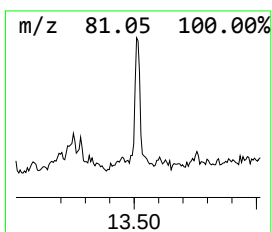
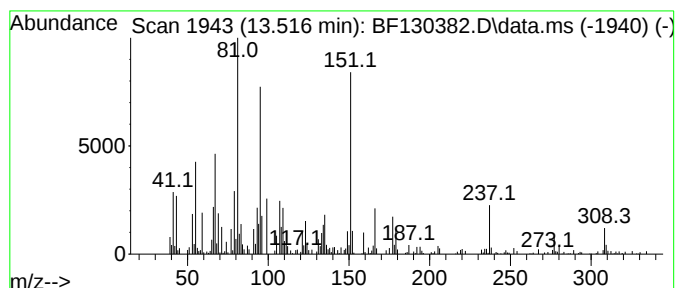
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.516 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.516	4.69 ng	190204	Chrysene-d12	13.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iododec-1-yne			264	C10H17I	067826-81-7	38
2	Butane-1,3-dione, 1-(pyrrol-2-yl)-			151	C8H9NO2	022441-25-4	25
3	Bicyclo[2.2.1]heptane, 2-(2-meth...			150	C11H18	061142-27-6	25
4	2-n-Heptylfuran			166	C11H18O	003777-71-7	18
5	5-Hydroxyadamantan-2-one			166	C10H14O2	020098-14-0	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130382.D
Acq On : 22 Sep 2022 18:43
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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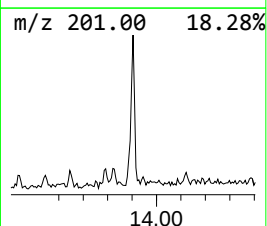
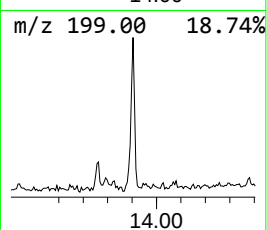
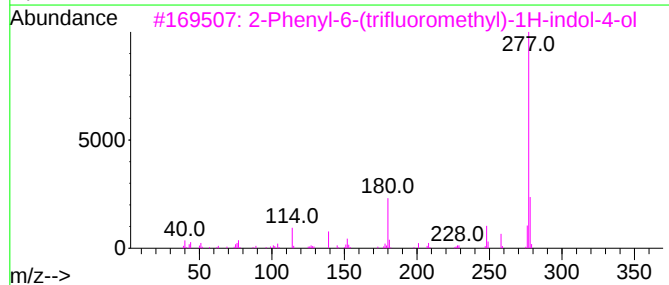
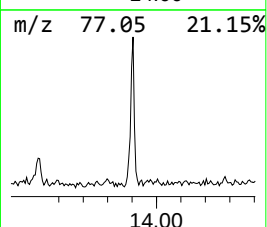
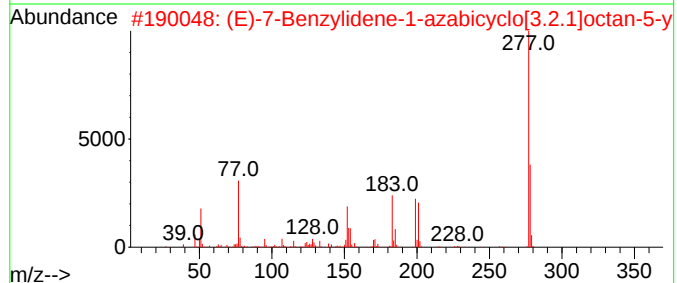
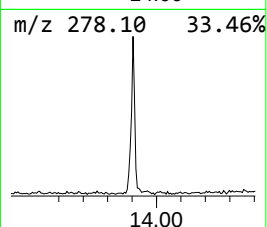
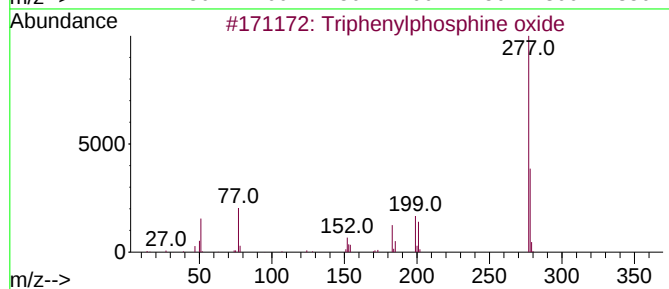
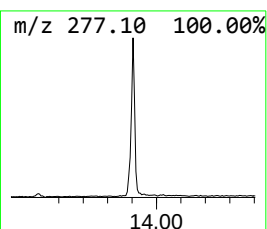
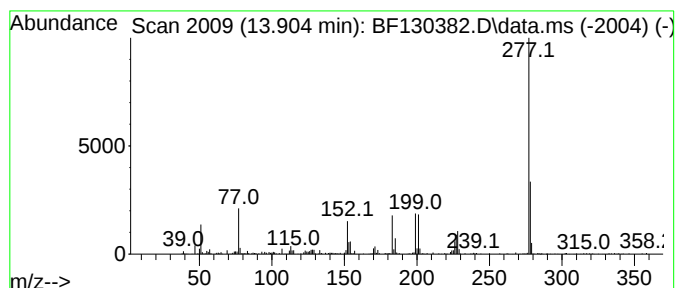
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triphenylphosphine oxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	6.85 ng	277905	Chrysene-d12	13.804

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	C15H19NO3S	1000483-83-4	62
3			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	38
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38
5			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130382.D
Acq On : 22 Sep 2022 18:43
Operator : CG\JU
Sample : N4752-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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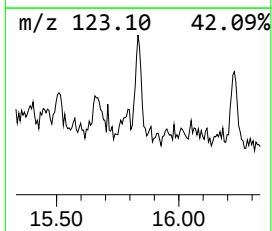
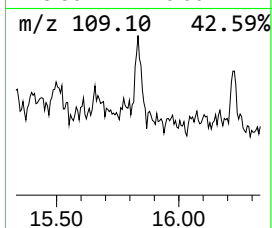
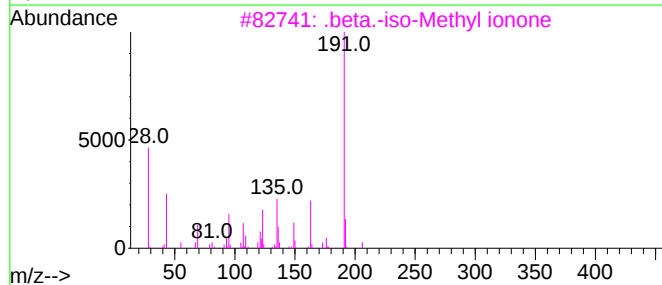
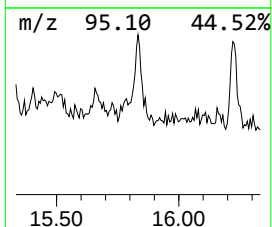
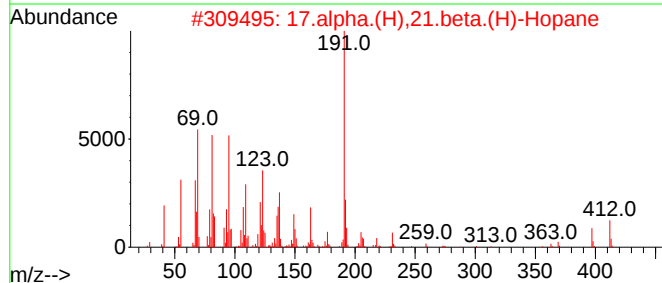
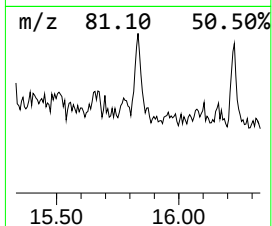
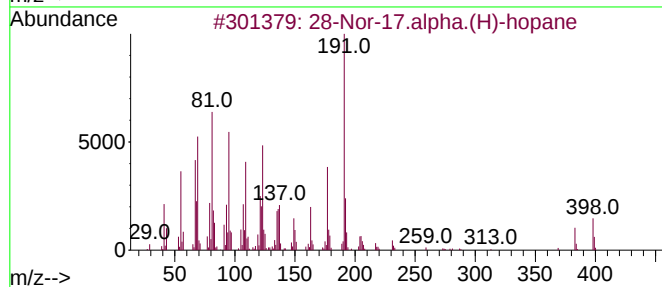
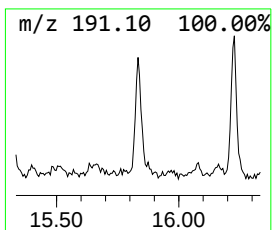
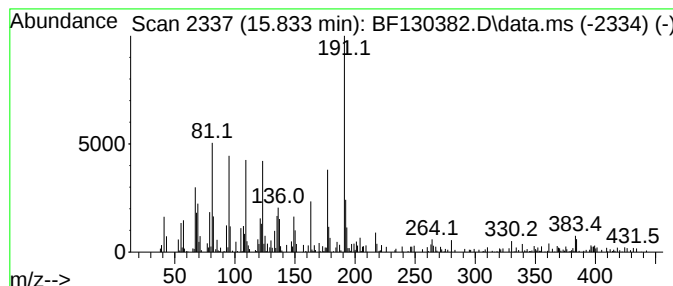
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 28-Nor-17.alpha.(H)-hopane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.833	11.94 ng	265386	Perylene-d12	15.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	83
2			17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	76
3			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
4			Fumaric acid, di(2-isopropoxyphe...	384	C22H24O6	1000344-85-0	27
5			2-Fluoro-5-(trifluoromethyl)benz...	339	C18H17F4NO	1000490-66-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130382.D
Acq On : 22 Sep 2022 18:43
Operator : CG\JU
Sample : N4752-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-07-092122

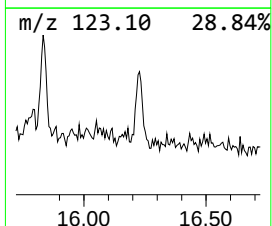
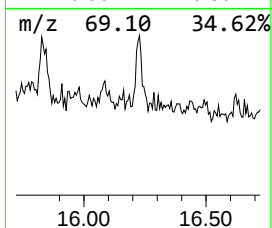
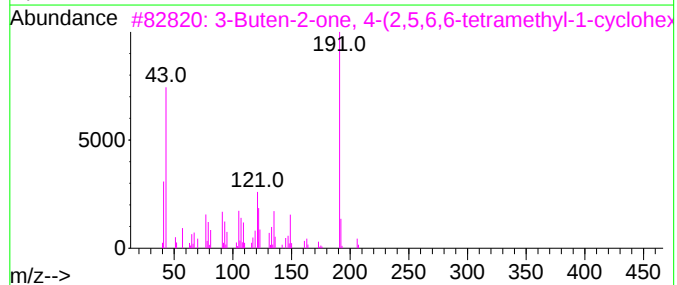
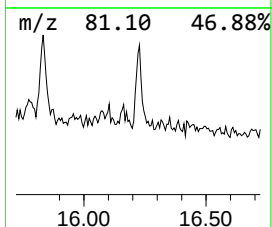
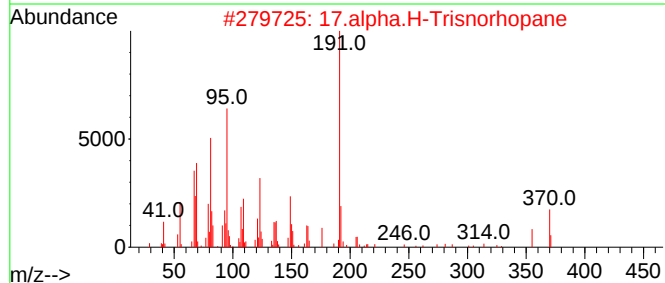
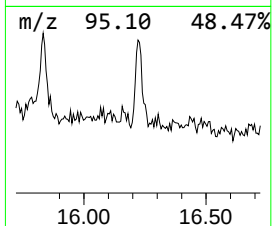
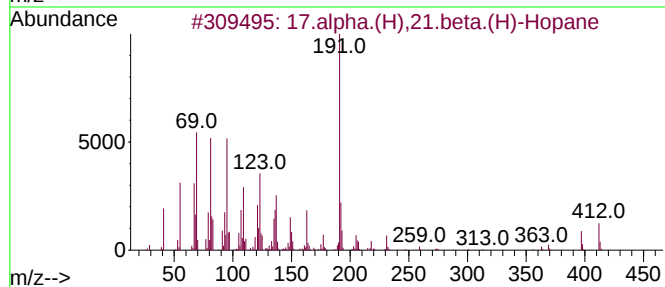
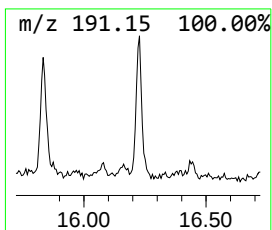
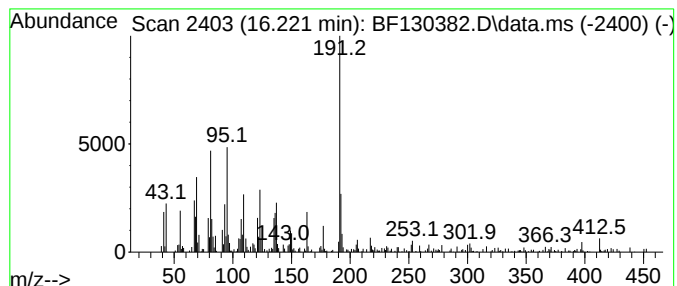
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.221	11.05 ng	245568	Perylene-d12	15.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	94
2			17.alpha.H-Trisnorhopane	370	C27H46	053584-59-1	90
3			3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	38
4			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
5			28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130382.D
Acq On : 22 Sep 2022 18:43
Operator : CG\JU
Sample : N4752-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-07-092122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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
Hexadecanoic ac...	11.575	98.2	ng	3348560	4	11.169	682148	20.0
n-Hexadecanoic ...	11.716	29.6	ng	1010380	4	11.169	682148	20.0
9,12-Octadecadi...	12.275	435.3	ng	14848100	4	11.169	682148	20.0
13-Octadecenoic...	12.298	245.9	ng	8385790	4	11.169	682148	20.0
Octadecanoic acid	12.498	3.7	ng	149219	5	13.804	811786	20.0
Methyl 9.cis.,1...	12.963	8.3	ng	336295	5	13.804	811786	20.0
11-Eicosenoic a...	13.010	4.8	ng	193847	5	13.804	811786	20.0
Eicosanoic acid...	13.086	5.2	ng	211897	5	13.804	811786	20.0
unknown13.516	13.516	4.7	ng	190204	5	13.804	811786	20.0
Triphenylphosph...	13.904	6.8	ng	277905	5	13.804	811786	20.0
28-Nor-17.alpha...	15.833	11.9	ng	265386	6	15.198	444455	20.0
17.alpha.(H),21...	16.221	11.1	ng	245568	6	15.198	444455	20.0