

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
 Data File : BF129492.D
 Acq On : 02 Aug 2022 01:12
 Operator : CG\JU
 Sample : N3979-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-06-072922

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-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129492.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.510	544	548	566	rBV	3131835	2784376	2.96%	1.514%
2	6.522	716	720	726	rBV	2892456	2486619	2.64%	1.353%
3	7.440	872	876	879	rBV	1855538	1557199	1.65%	0.847%
4	9.228	1176	1180	1184	rBV	2766969	2401427	2.55%	1.306%
5	10.704	1428	1431	1435	rBV	1803986	1472657	1.56%	0.801%
6	11.404	1546	1550	1552	rBV	1093929	955965	1.02%	0.520%
7	11.810	1611	1619	1621	rBV	15825642	25634778	27.23%	13.943%
8	11.969	1638	1646	1651	rVV2	2853006	4720939	5.01%	2.568%
9	12.022	1651	1655	1663	rVV3	584884	1179237	1.25%	0.641%
10	12.551	1724	1745	1746	rBV2	22332077	94142924	100.00%	51.206%
11	12.610	1752	1755	1757	rVB	13021362	14021833	14.89%	7.627%
12	12.657	1757	1763	1773	rVB3	5148721	12444171	13.22%	6.769%
13	12.869	1795	1799	1807	rVB2	1412404	2727840	2.90%	1.484%
14	13.004	1817	1822	1825	rBV	2913825	3099297	3.29%	1.686%
15	13.181	1847	1852	1855	rBV5	589009	1111493	1.18%	0.605%
16	13.228	1858	1860	1867	rVB2	1608314	2186645	2.32%	1.189%
17	13.304	1869	1873	1876	rBV2	2327675	2475259	2.63%	1.346%
18	13.469	1897	1901	1905	rVB2	827320	1002065	1.06%	0.545%
19	13.739	1943	1947	1953	rVB3	843133	1221408	1.30%	0.664%
20	13.975	1983	1987	1990	rBV	2518826	2322684	2.47%	1.263%
21	14.051	1996	2000	2003	rBV2	1224554	1876166	1.99%	1.020%
22	14.080	2003	2005	2012	rVB	1041382	1029030	1.09%	0.560%
23	15.104	2175	2179	2182	rBV	674535	996123	1.06%	0.542%

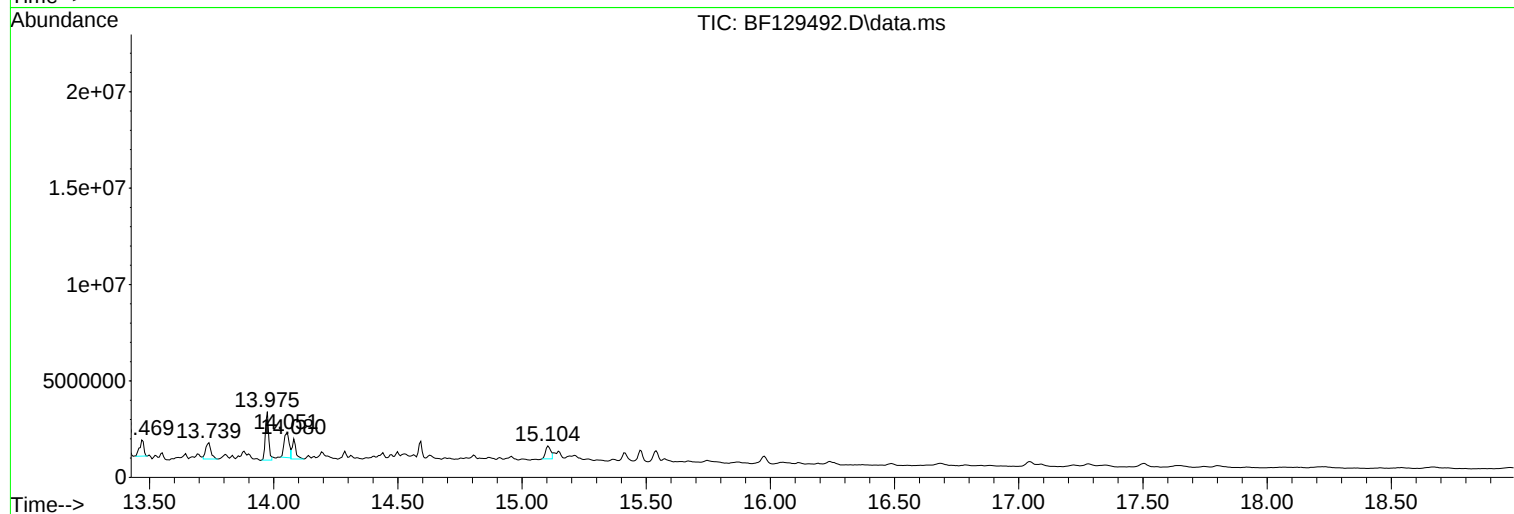
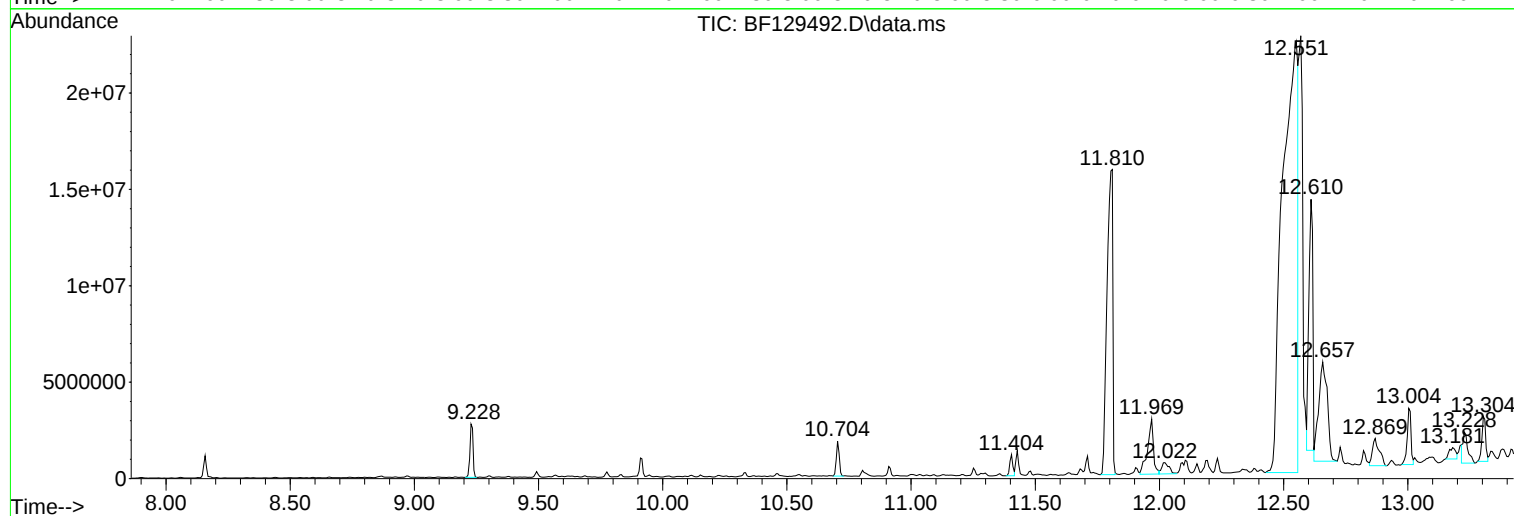
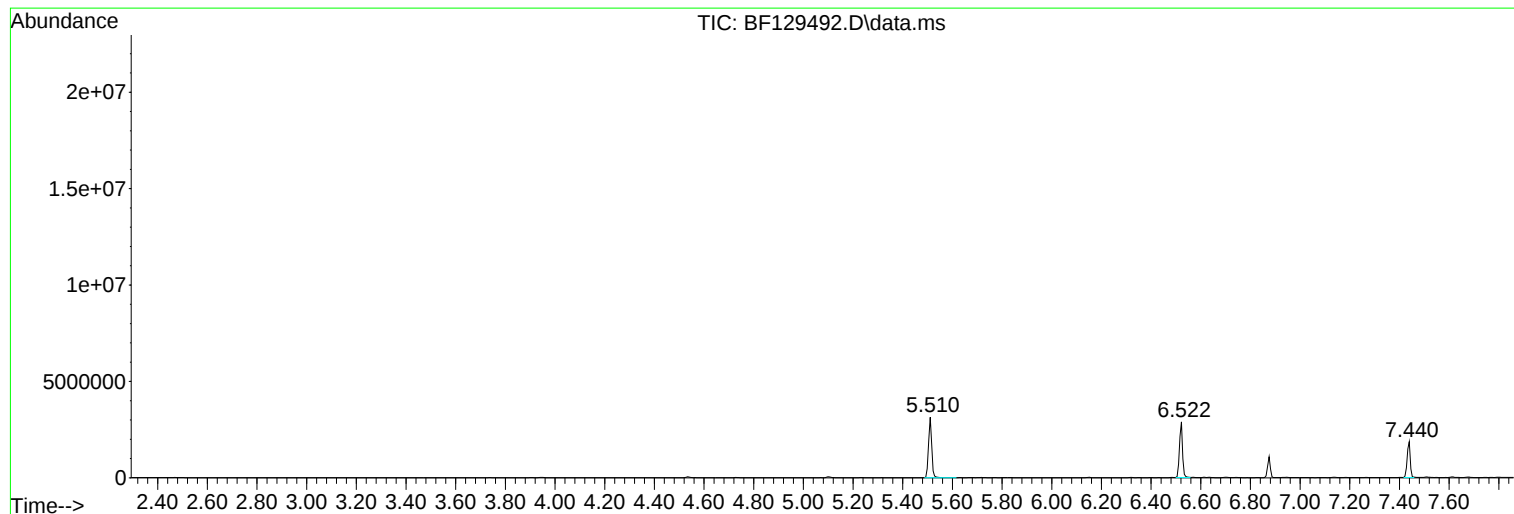
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ClientSampleId :
TR-06-072922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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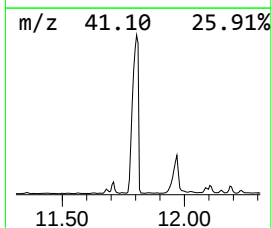
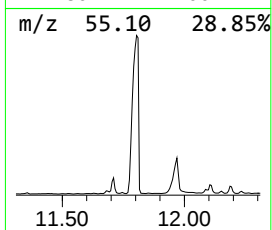
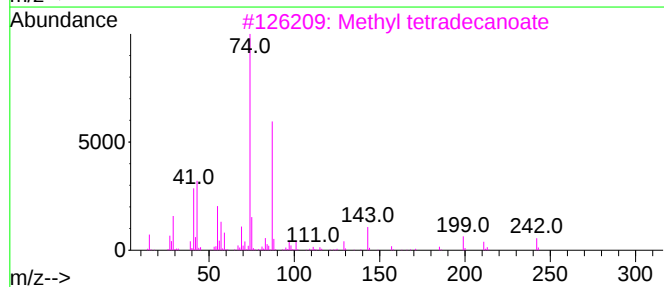
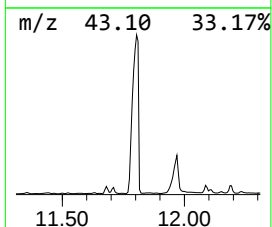
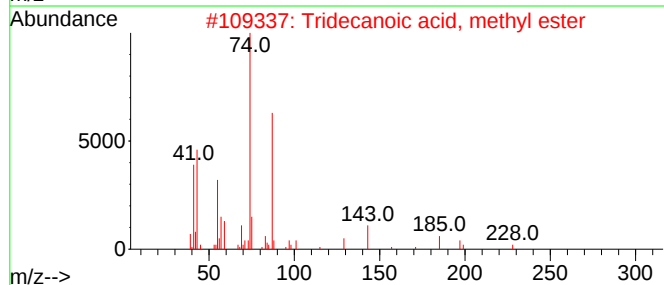
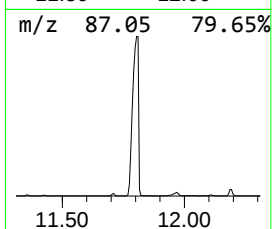
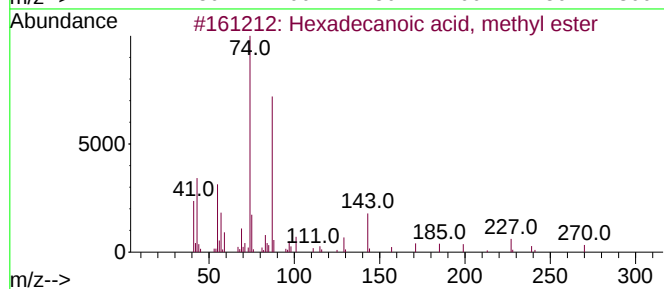
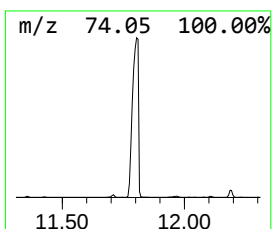
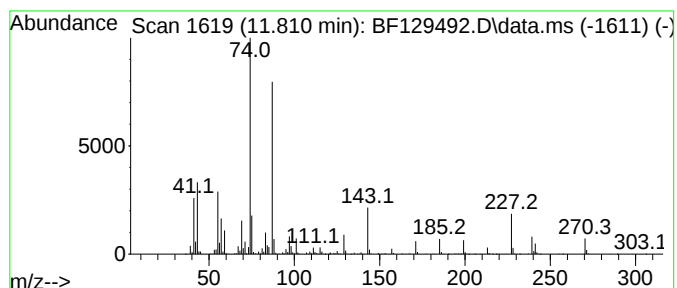
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.810	536.31 ng	25634800	Phenanthrene-d10		11.404	
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	Methyl tetradecanoate		242	C15H30O2	000124-10-7	87
4	Methyl 9-methyltetradecanoate		256	C16H32O2	213617-69-7	87
5	Methyl 11-methyl-dodecanoate		228	C14H28O2	1000336-45-1	80



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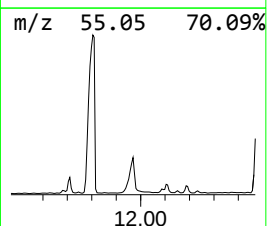
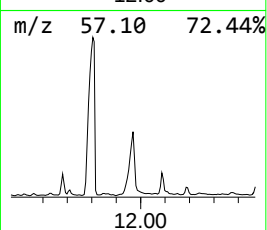
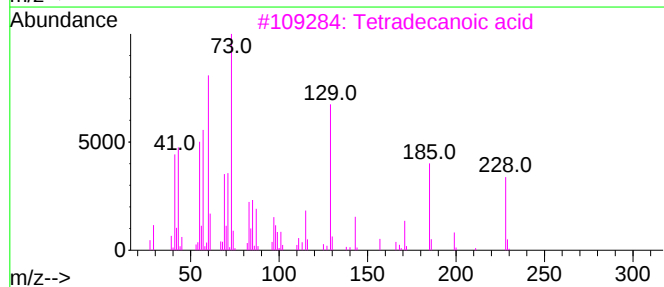
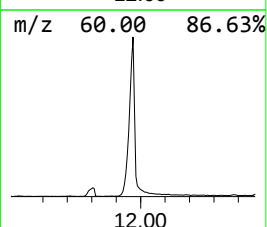
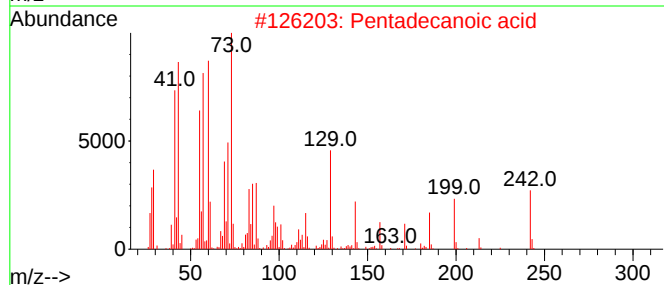
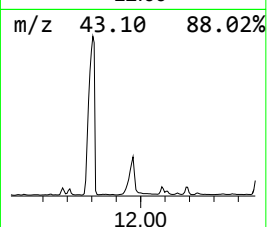
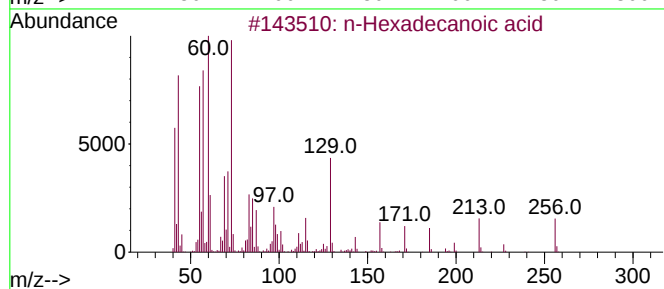
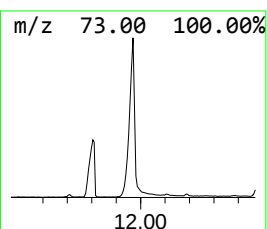
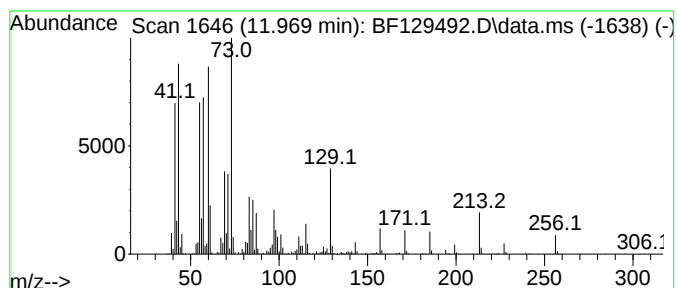
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.969	98.77 ng	4720940	Phenanthrene-d10		11.404	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	90
4	Tridecanoic acid		214	C13H26O2	000638-53-9	72
5	Dodecanoic acid		200	C12H24O2	000143-07-7	59



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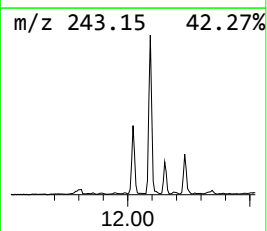
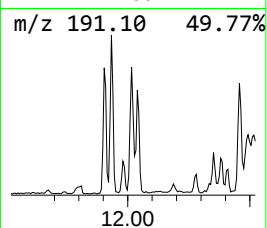
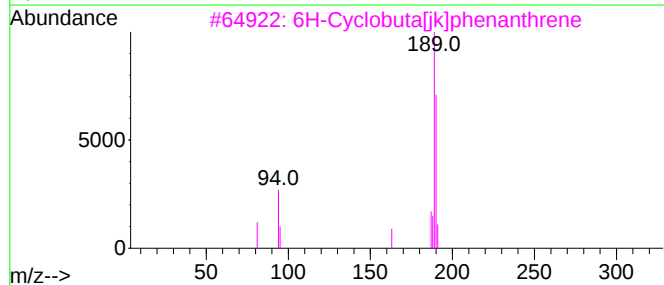
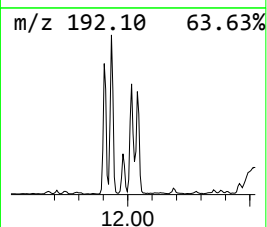
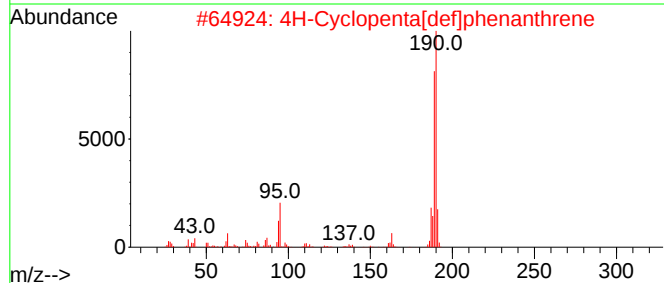
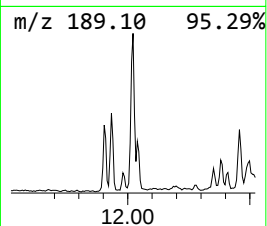
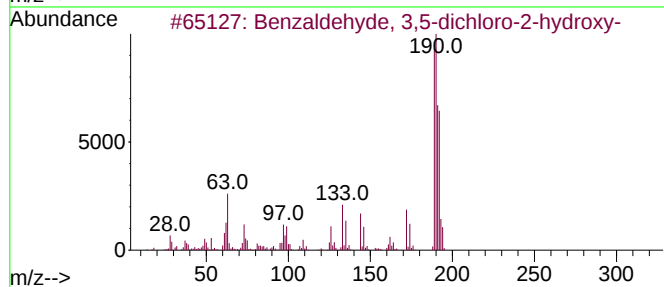
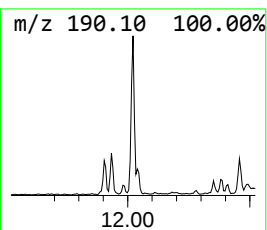
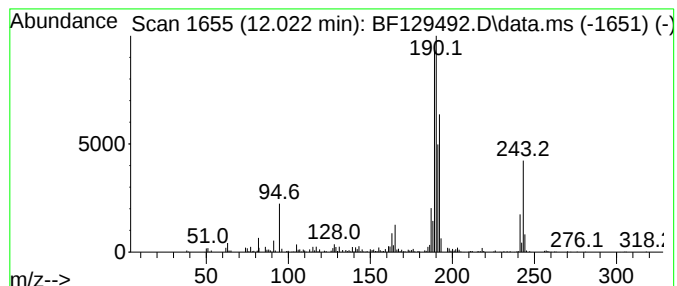
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzaldehyde, 3,5-dichloro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.022	24.67 ng	1179240	Phenanthrene-d10		11.404	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...		190	C7H4Cl2O2	000090-60-8	53
2	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	49
3	6H-Cyclobuta[jk]phenanthrene		190	C15H10	083469-43-6	47
4	4,6-Dichloro-2-ethylpyrimidin-5-...		191	C6H7Cl2N3	006237-96-3	25
5	5H-Dibenzo[a,d]cycloheptene		192	C15H12	000256-81-5	11



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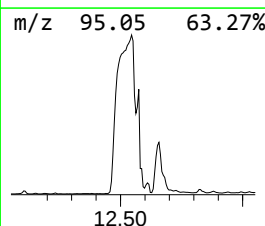
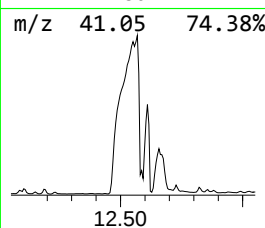
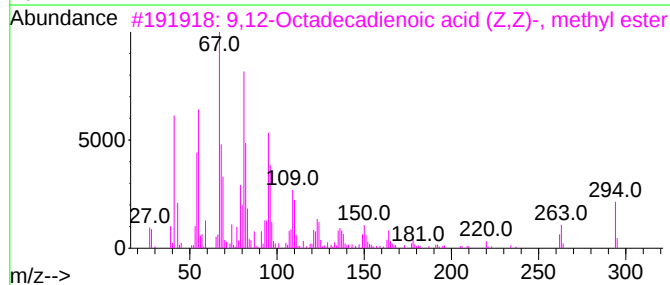
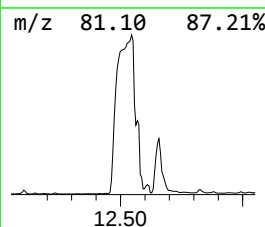
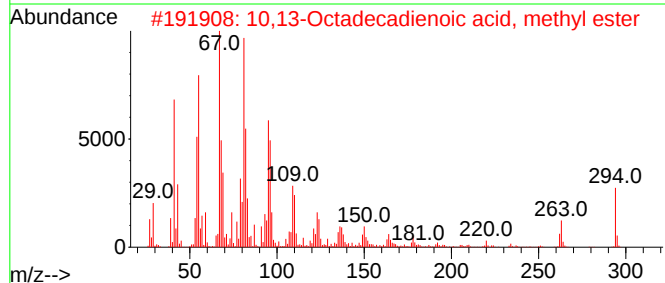
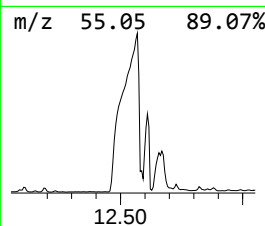
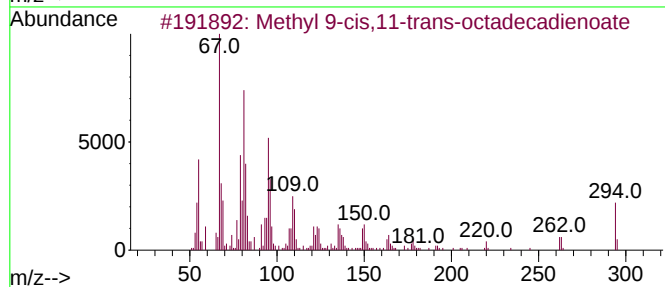
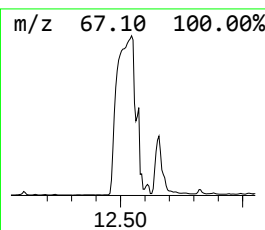
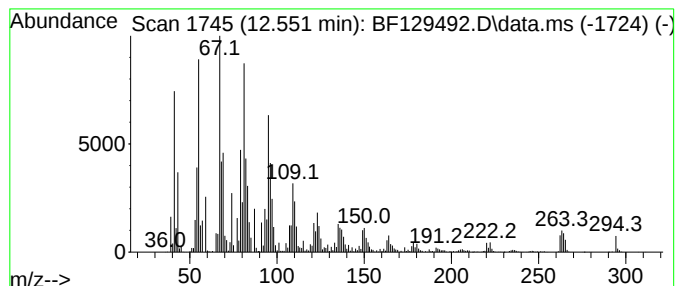
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Peak Number 4 Methyl 9-cis,11-trans-octad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	1969.59 ng	94142900	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
2			10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99



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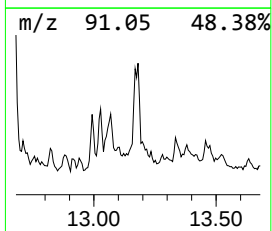
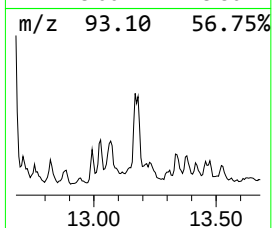
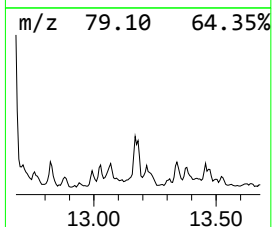
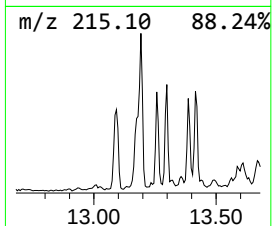
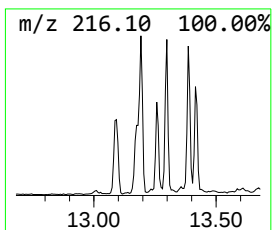
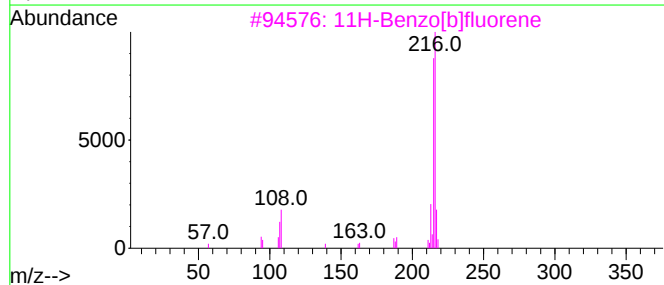
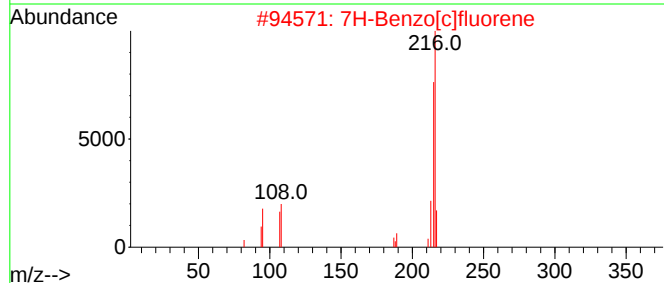
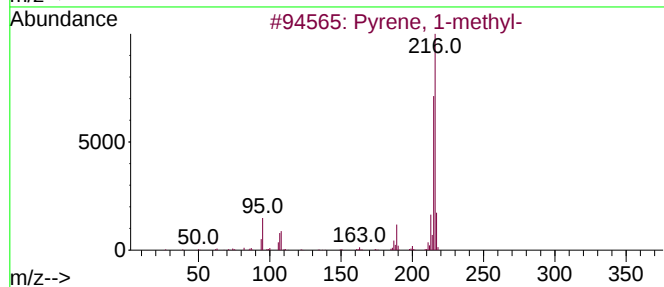
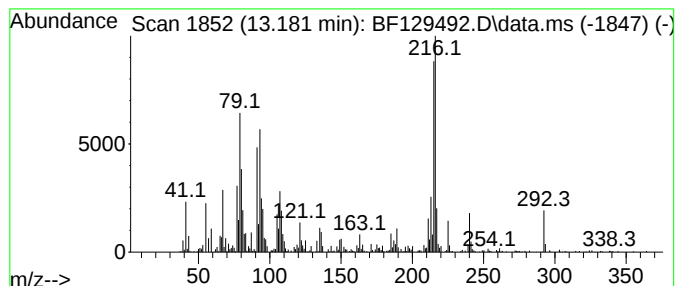
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Peak Number 5 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.181	11.85 ng	1111490	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
2			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	64
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	60
5			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	60



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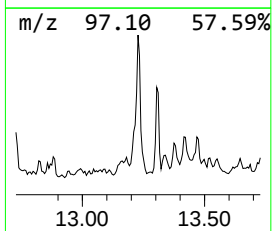
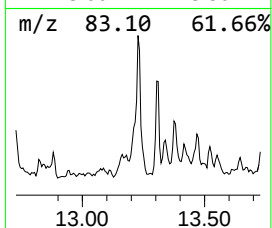
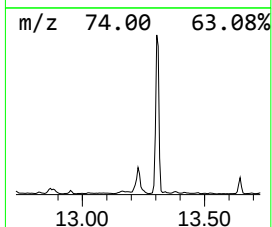
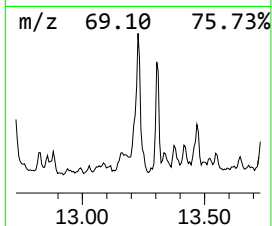
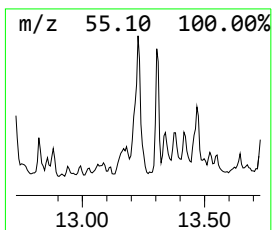
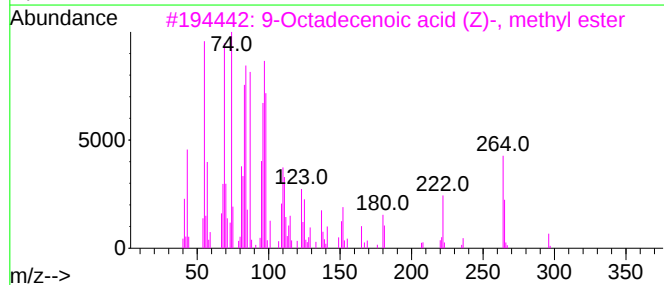
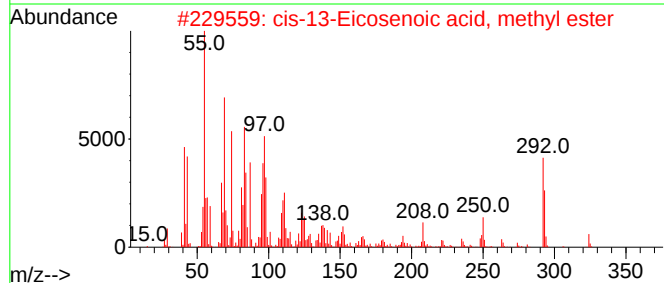
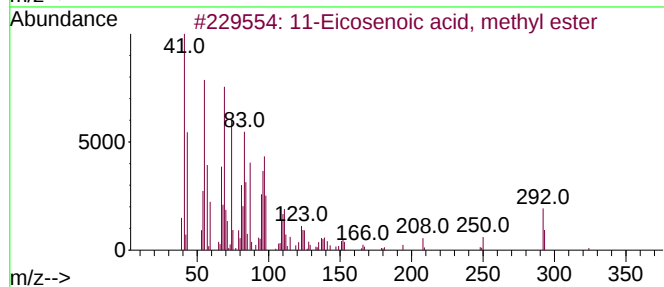
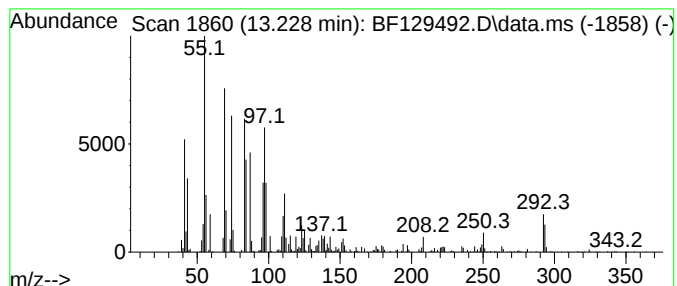
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 11-Eicosenoic acid, methyl ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.228	23.31 ng	2186650	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	94
2			cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	93
3			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	59
4			cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	55
5			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
Data File : BF129492.D
Acq On : 02 Aug 2022 01:12
Operator : CG\JU
Sample : N3979-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-072922

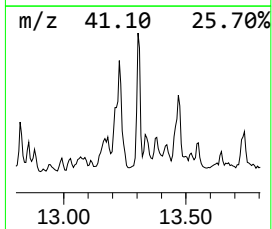
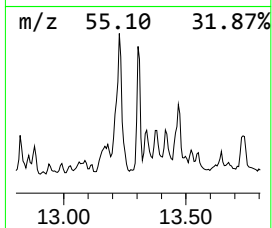
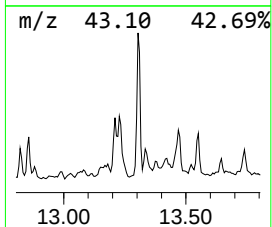
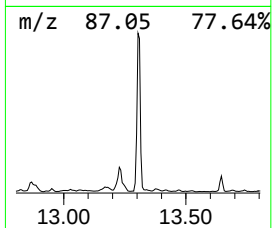
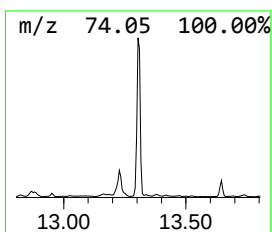
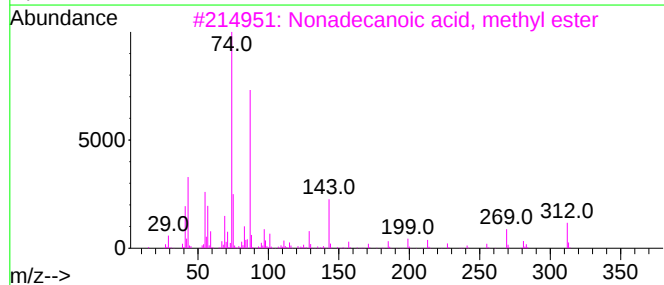
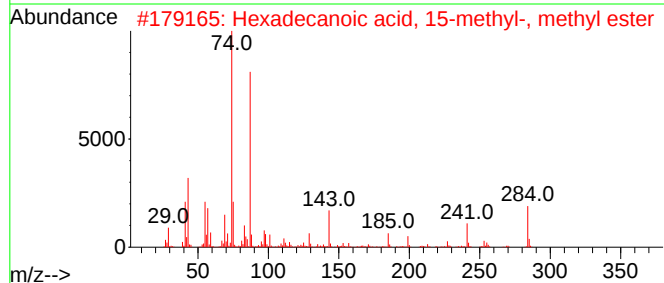
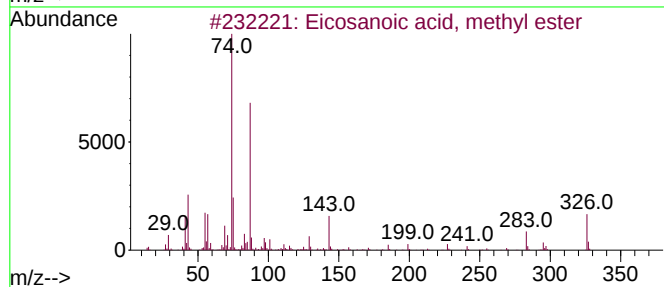
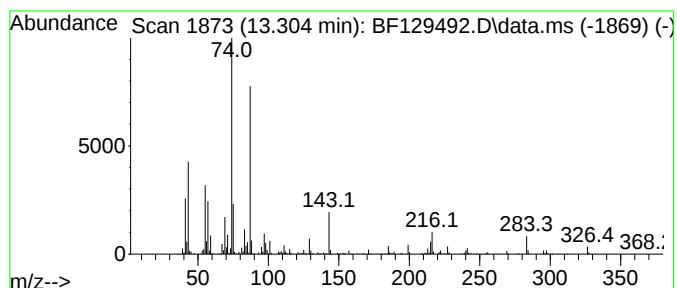
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.304	26.39 ng	2475260	Chrysene-d12	14.057

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	97
3			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	90
4			Methyl stearate	298	C19H38O2	000112-61-8	90
5			Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
Data File : BF129492.D
Acq On : 02 Aug 2022 01:12
Operator : CG\JU
Sample : N3979-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

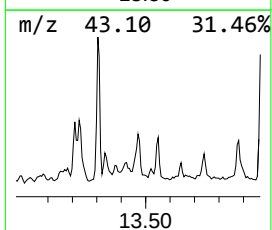
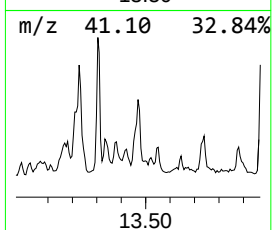
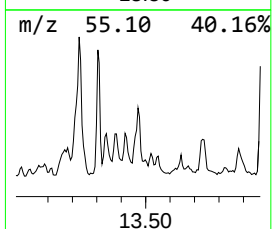
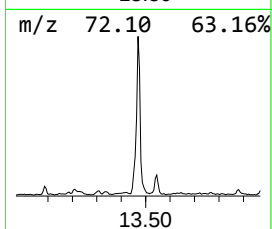
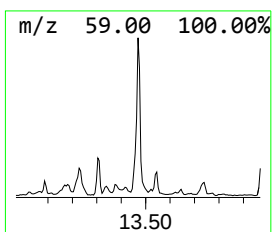
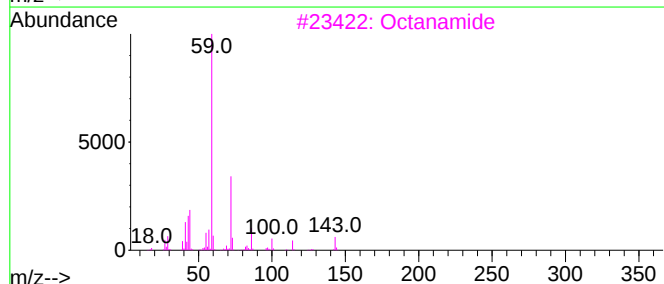
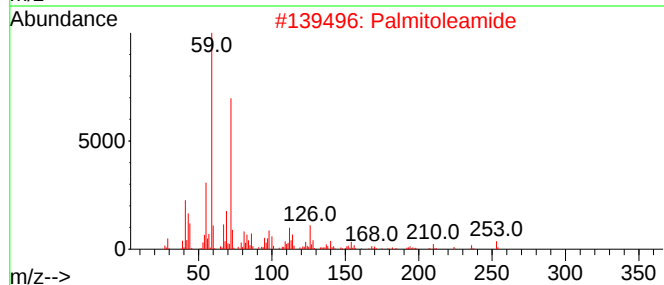
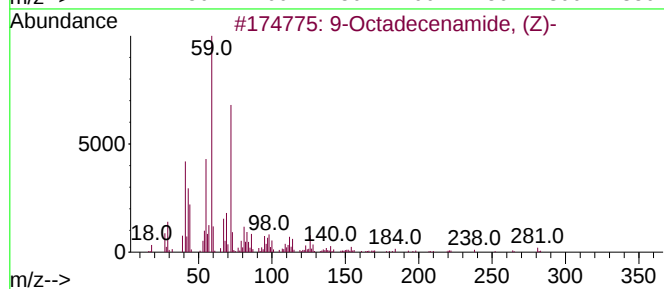
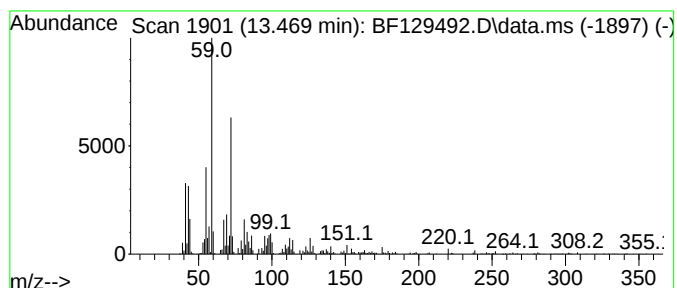
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BNA_F
ClientSampleId :
TR-06-072922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.469	10.68 ng	1002070	Chrysene-d12	14.057	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2	Palmitoleamide	253	C16H31NO	106010-22-4	80
3	Octanamide	143	C8H17NO	000629-01-6	53
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
Data File : BF129492.D
Acq On : 02 Aug 2022 01:12
Operator : CG\JU
Sample : N3979-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-072922

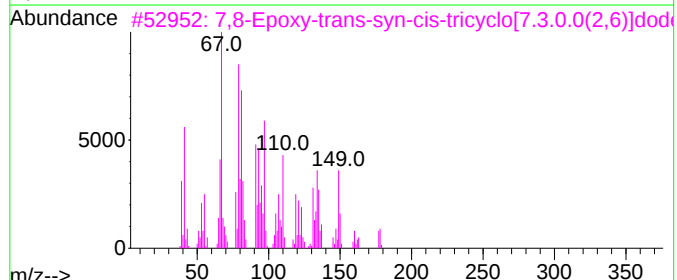
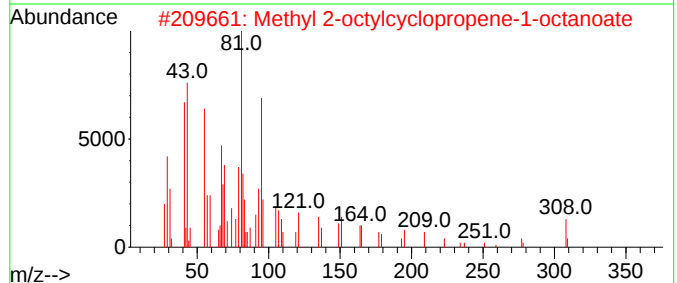
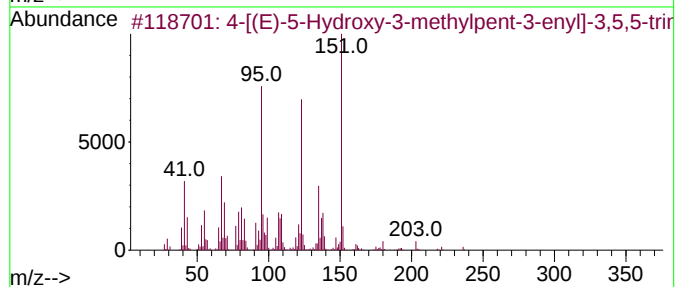
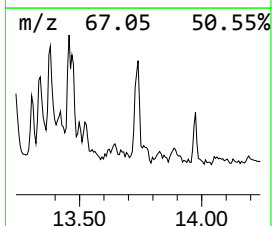
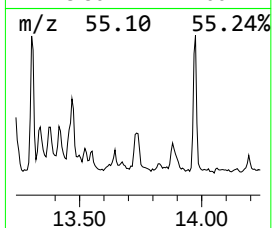
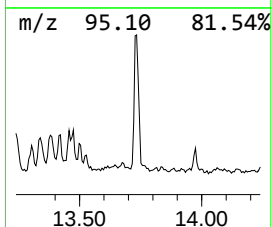
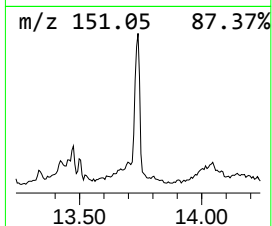
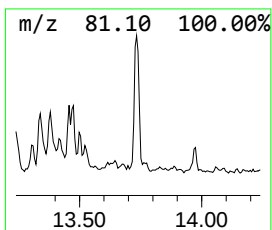
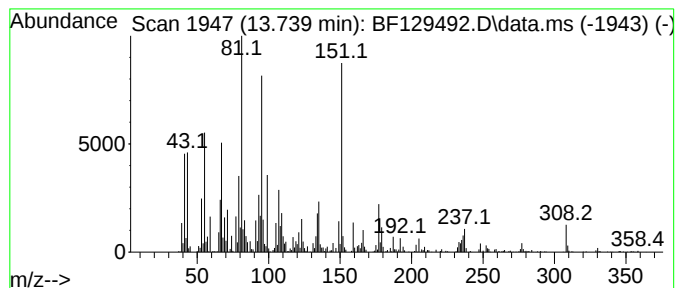
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.739 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	13.02 ng	1221410	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-[(E)-5-Hydroxy-3-methylpent-3-...	236	C15H24O2	1083195-46-3	46		
2	Methyl 2-octylcyclopropene-1-oct...	308	C20H36O2	003220-60-8	15		
3	7,8-Epoxy-trans-syn-cis-tricyclo...	178	C12H18O	057366-09-3	15		
4	Bicyclo[2.2.1]heptane, 2-butyl-	152	C11H20	061177-16-0	11		
5	Isoborneol	154	C10H18O	000124-76-5	11		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
Data File : BF129492.D
Acq On : 02 Aug 2022 01:12
Operator : CG\JU
Sample : N3979-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-072922

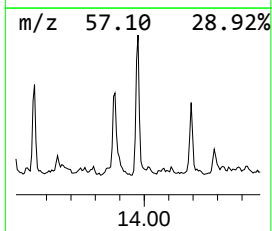
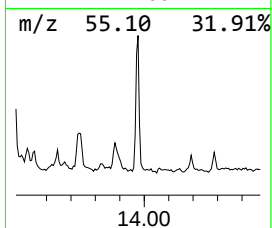
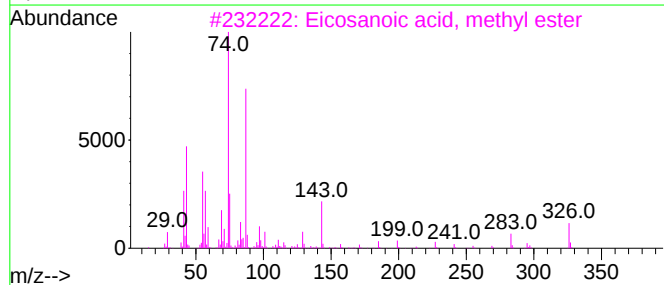
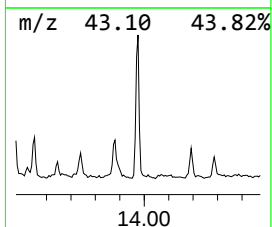
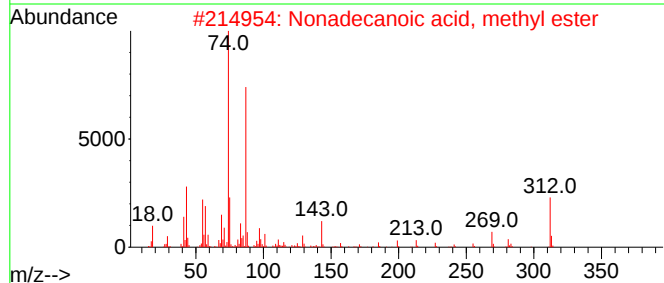
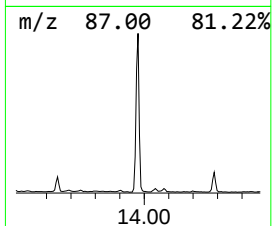
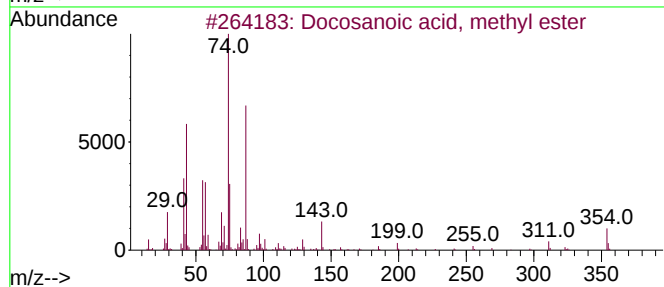
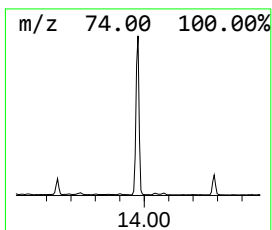
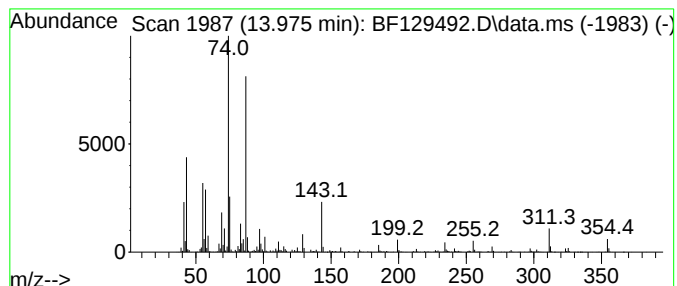
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.975	24.76 ng	2322680	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	99
2			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	95
3			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	90
4			Silane, methylvinyl(cis-2-methyl...	326	C19H38O2Si	1000421-05-3	89
5			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
Data File : BF129492.D
Acq On : 02 Aug 2022 01:12
Operator : CG\JU
Sample : N3979-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-072922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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
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n-Hexadecanoic ...	11.969	98.8	ng	4720940	4	11.404	955965	20.0
Benzaldehyde, 3...	12.022	24.7	ng	1179240	4	11.404	955965	20.0
Methyl 9-cis,11...	12.551	1969.6	ng	94142900	4	11.404	955965	20.0
Pyrene, 1-methyl-	13.181	11.9	ng	1111490	5	14.057	1876170	20.0
11-Eicosenoic a...	13.228	23.3	ng	2186650	5	14.057	1876170	20.0
Eicosanoic acid...	13.304	26.4	ng	2475260	5	14.057	1876170	20.0
9-Octadecenamid...	13.469	10.7	ng	1002070	5	14.057	1876170	20.0
unknown13.739	13.739	13.0	ng	1221410	5	14.057	1876170	20.0
Docosanoic acid...	13.975	24.8	ng	2322680	5	14.057	1876170	20.0