

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
 Data File : BF127771.D
 Acq On : 12 Apr 2022 21:29
 Operator : CG\JU
 Sample : N2365-01 2X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-04-041122

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-BF040622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127771.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.569	554	558	562	rBV	1576291	1433288	2.42%	1.214%
2	6.569	724	728	732	rBV	1494950	1387445	2.34%	1.175%
3	6.957	790	794	797	rVB	959038	756157	1.27%	0.640%
4	7.516	885	889	892	rBV	1154744	924479	1.56%	0.783%
5	8.239	1009	1012	1015	rVB	1122020	854036	1.44%	0.723%
6	9.310	1191	1194	1198	rVB	2021046	1605216	2.71%	1.359%
7	9.998	1307	1311	1314	rVB	1087528	910290	1.53%	0.771%
8	10.786	1442	1445	1448	rVB	935640	824897	1.39%	0.699%
9	11.486	1561	1564	1567	rBV	979985	851157	1.44%	0.721%
10	11.892	1626	1633	1636	rBV	12059964	19235003	32.43%	16.289%
11	12.039	1650	1658	1666	rBV	1682244	2550863	4.30%	2.160%
12	12.633	1743	1759	1760	rBV4	14434256	59309403	100.00%	50.227%
13	12.698	1766	1770	1772	rVB	9756205	9170360	15.46%	7.766%
14	12.733	1772	1776	1778	rBV	3408126	4152201	7.00%	3.516%
15	13.092	1833	1837	1839	rVB	1625843	1403998	2.37%	1.189%
16	13.321	1870	1876	1882	rVB2	1213065	2109621	3.56%	1.787%
17	13.398	1885	1889	1892	rVV	1624954	1514671	2.55%	1.283%
18	13.427	1892	1894	1899	rVV3	1282905	1653103	2.79%	1.400%
19	13.469	1899	1901	1905	rVV	1185965	1417054	2.39%	1.200%
20	13.510	1906	1908	1912	rVV3	461185	628411	1.06%	0.532%
21	13.557	1912	1916	1920	rVV2	466616	757512	1.28%	0.642%
22	13.616	1923	1926	1929	rVV	735904	809033	1.36%	0.685%
23	13.827	1957	1962	1965	rBV2	500363	669209	1.13%	0.567%
24	14.063	1999	2002	2006	rBV	1402218	1270296	2.14%	1.076%
25	14.139	2011	2015	2018	rBV2	997288	1018505	1.72%	0.863%
26	15.663	2269	2274	2283	rVB	540141	867457	1.46%	0.735%

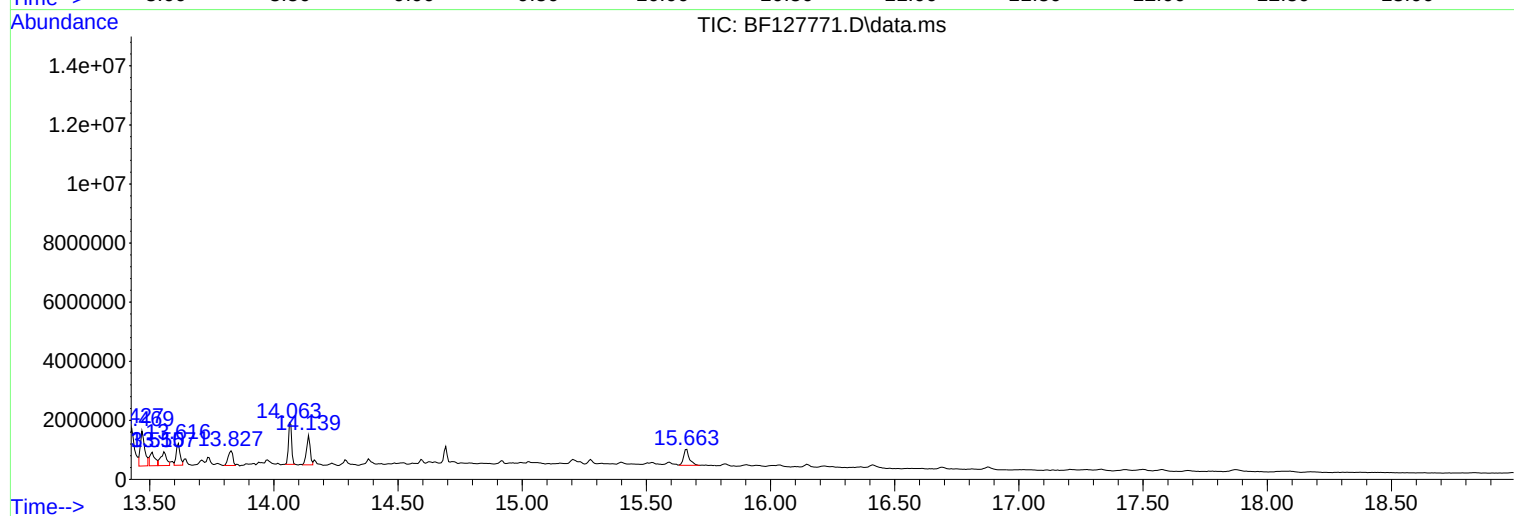
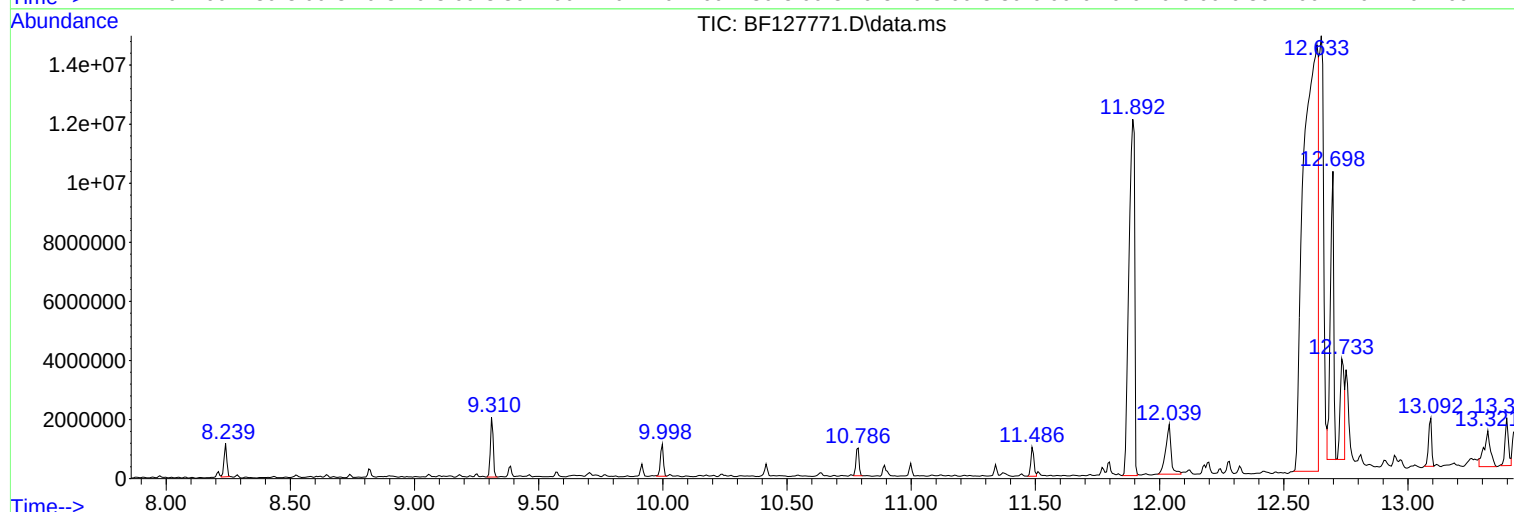
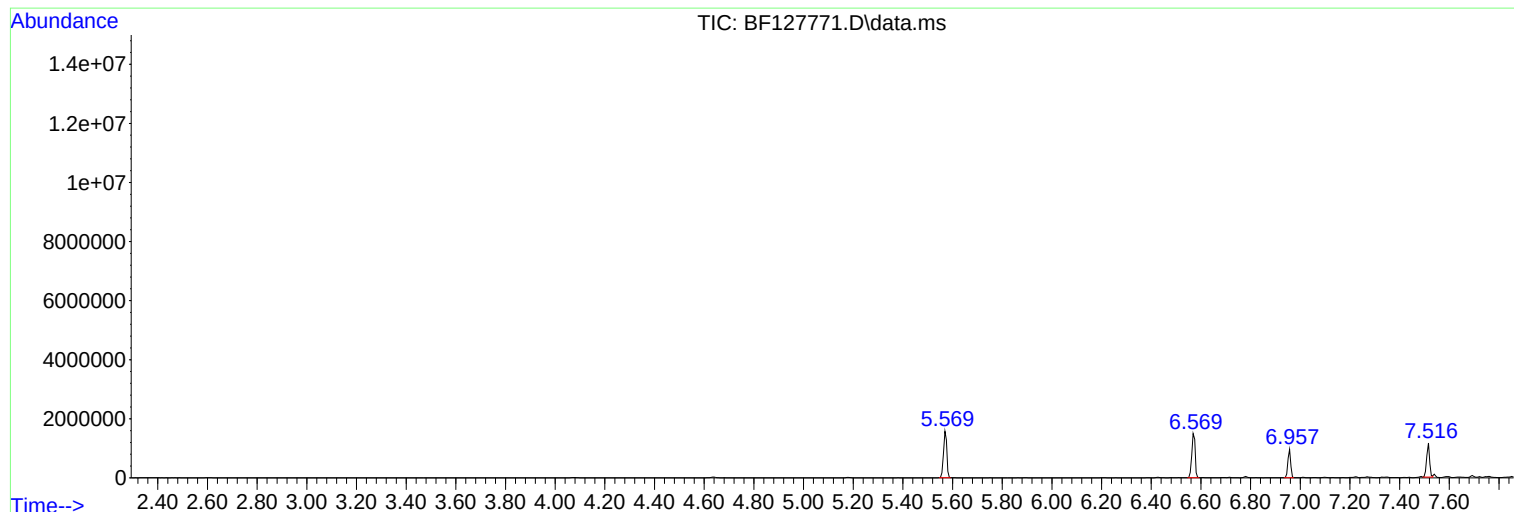
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Instrument :
BNA_F
ClientSampleId :
TR-04-041122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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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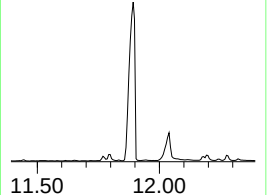
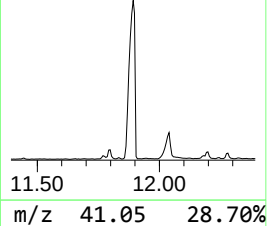
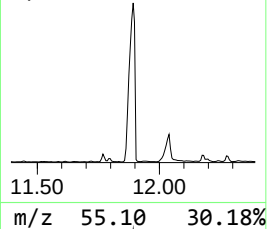
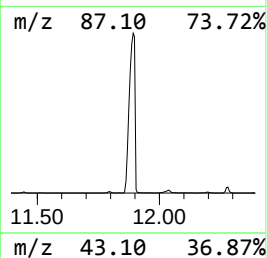
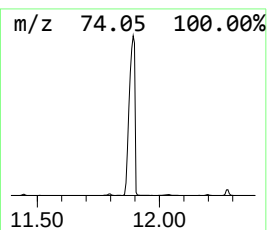
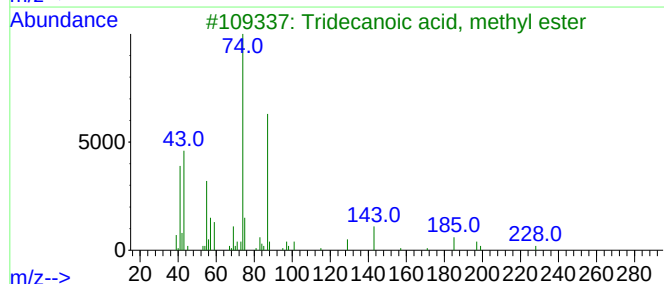
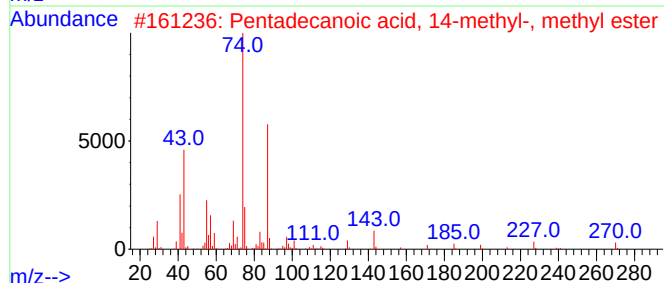
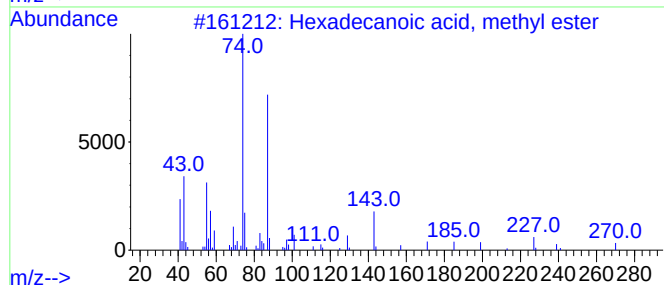
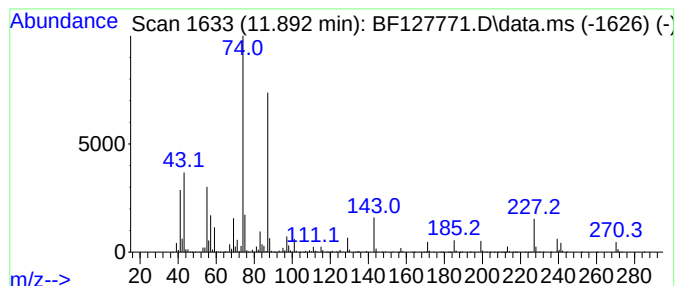
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
11.892	451.97 ng	19235000	Phenanthrene-d10		11.486	
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	96
3	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	91
4	Methyl tetradecanoate		242	C15H30O2	000124-10-7	87
5	Decanoic acid, methyl ester		186	C11H22O2	000110-42-9	87



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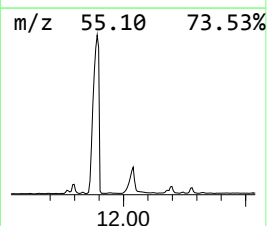
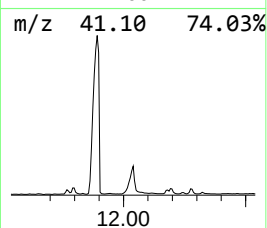
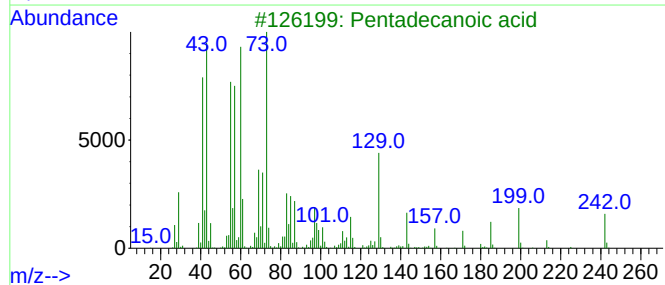
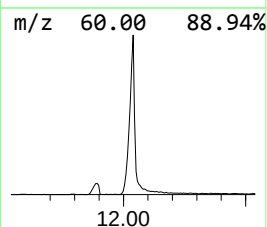
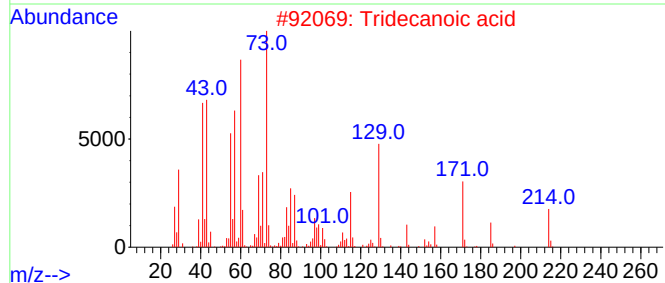
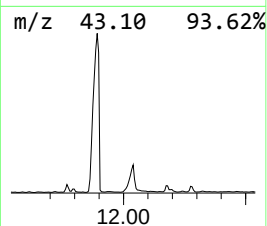
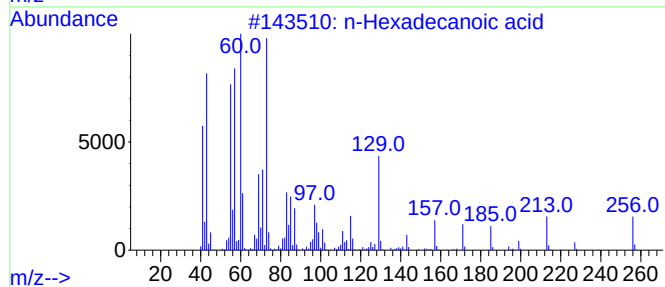
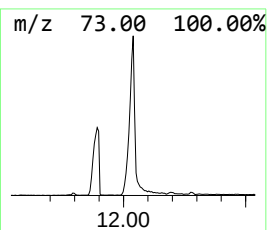
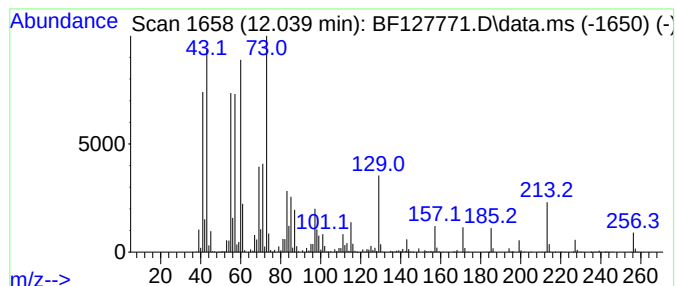
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	59.94 ng	2550860	Phenanthrene-d10	11.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64



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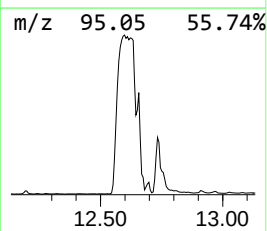
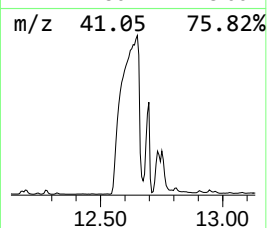
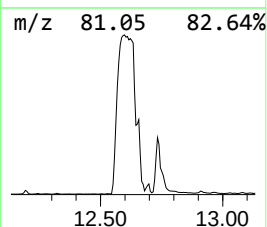
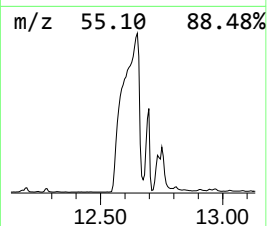
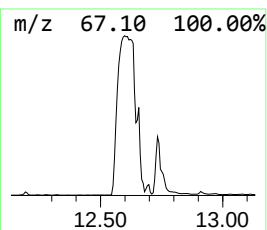
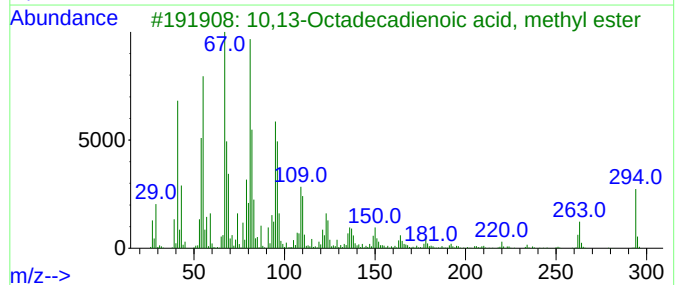
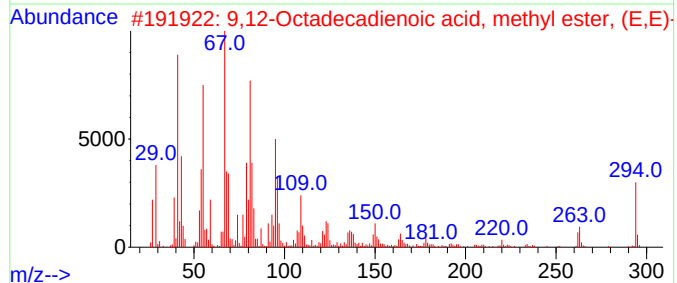
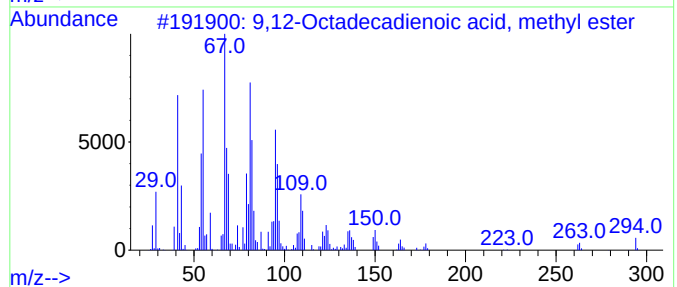
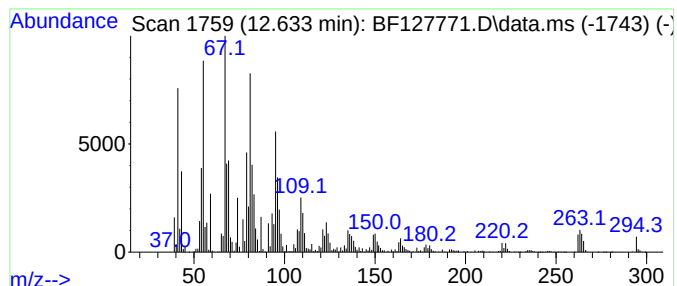
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	1393.62 ng	59309400	Phenanthrene-d10	11.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99		
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99		
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99		
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99		
5	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	98		



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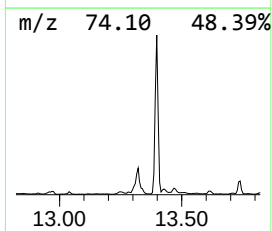
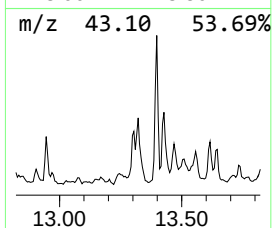
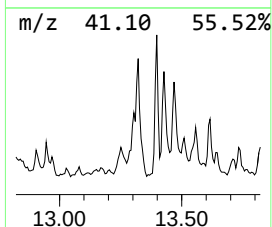
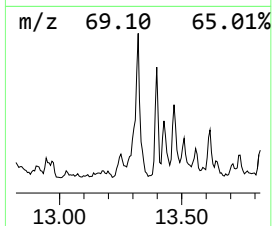
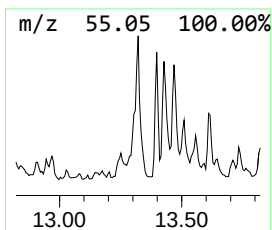
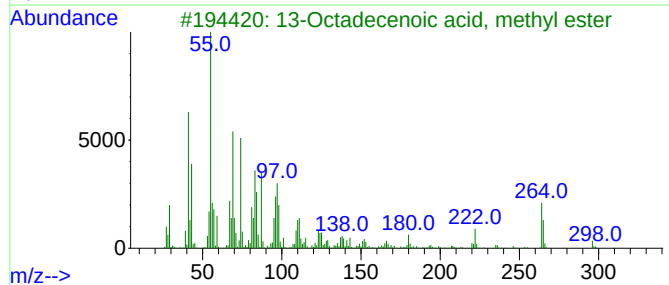
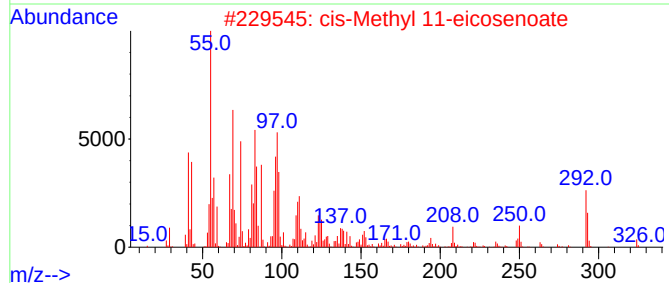
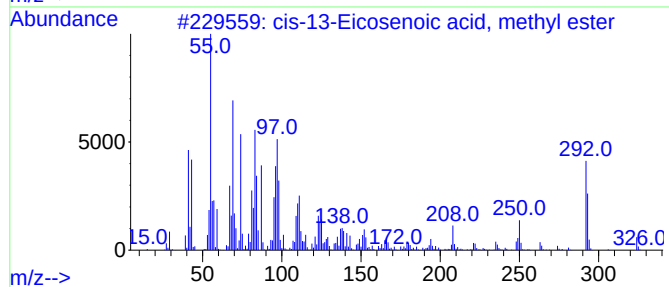
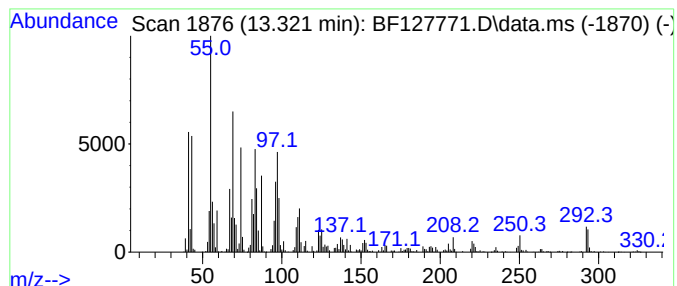
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 cis-13-Eicosenoic acid, met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.322	41.43 ng	2109620	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	94
2			cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	91
3			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	87
4			cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	87
5			Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	83



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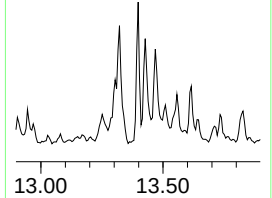
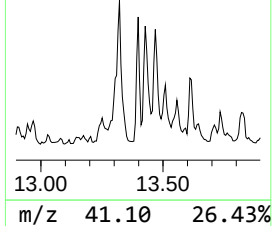
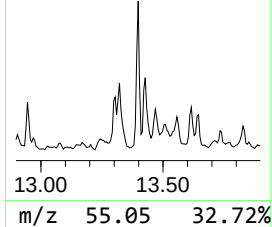
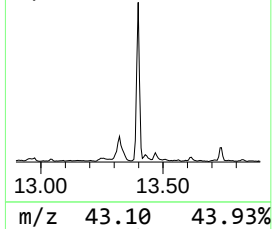
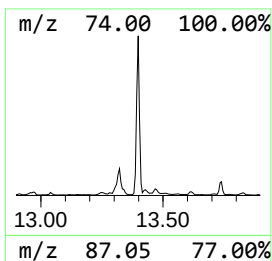
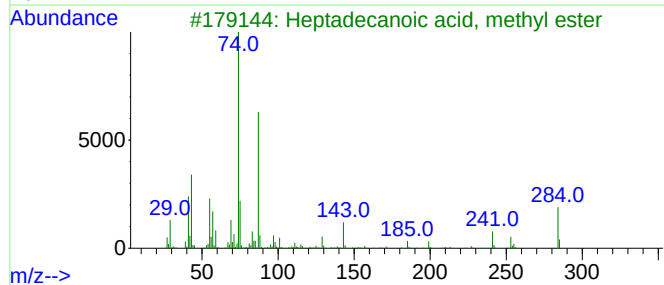
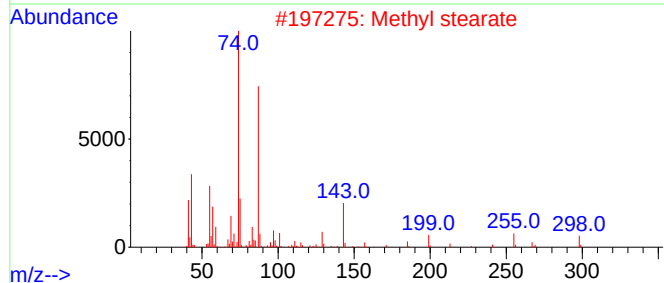
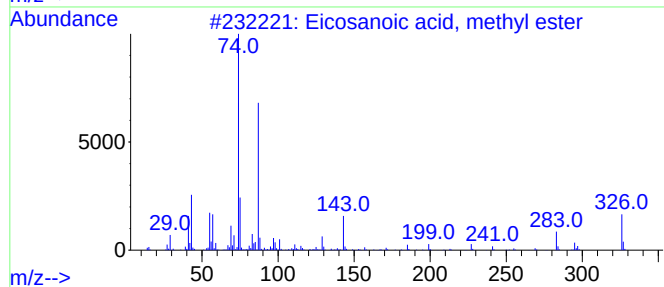
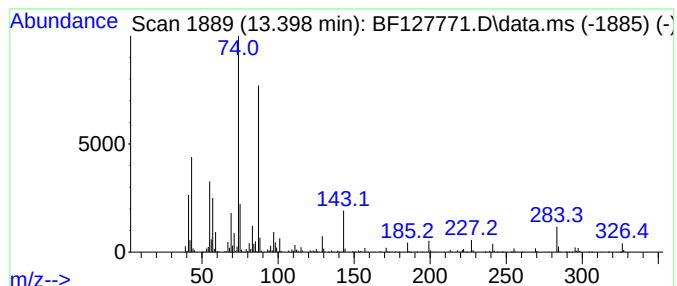
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Peak Number 5 Eicosanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.398	29.74 ng	1514670	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2			Methyl stearate	298	C19H38O2	000112-61-8	93
3			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
4			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
5			Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	90



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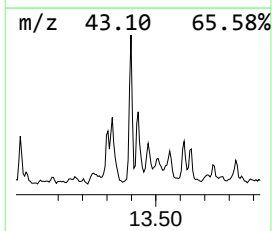
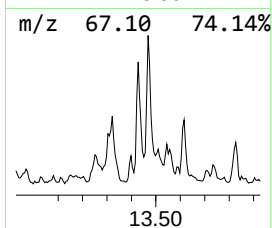
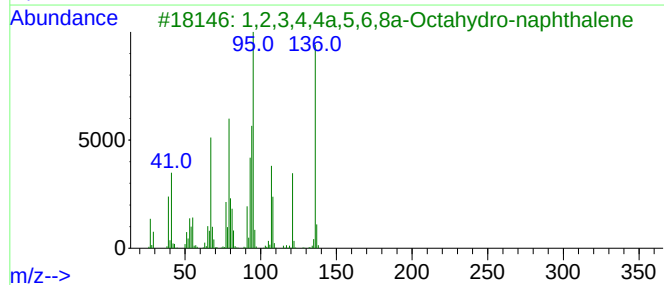
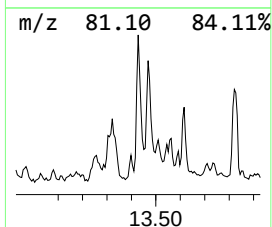
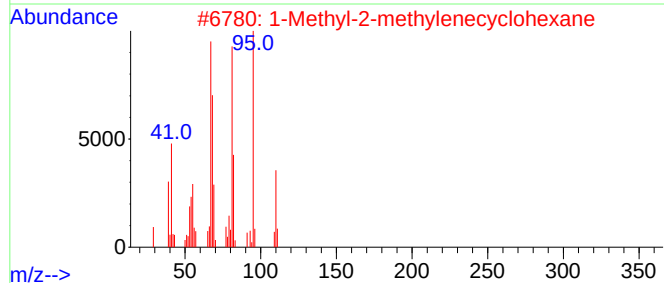
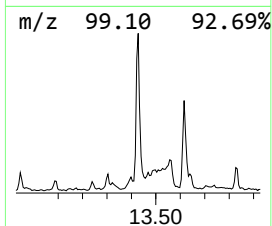
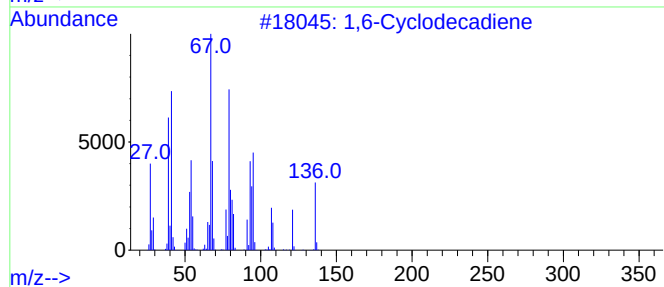
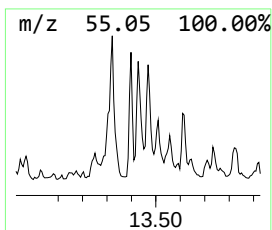
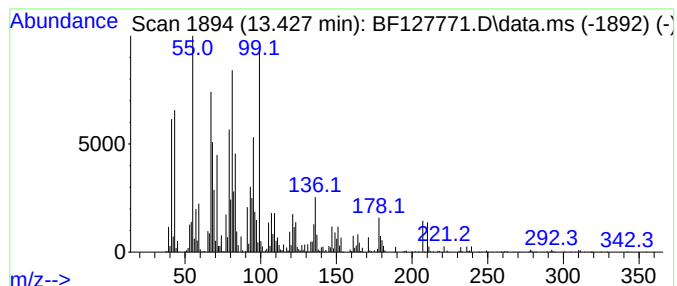
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,6-Cyclodecadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	32.46 ng	1653100	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,6-Cyclodecadiene	136	C10H16	007049-13-0	56
2			1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	50
3			1,2,3,4,4a,5,6,8a-Octahydro-naph...	136	C10H16	031244-58-3	50
4			Z-1,6-Tridecadiene	180	C13H24	1000130-98-3	46
5			1,5-Cyclodecadiene, (E,Z)-	136	C10H16	001124-78-3	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
Data File : BF127771.D
Acq On : 12 Apr 2022 21:29
Operator : CG\JU
Sample : N2365-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-041122

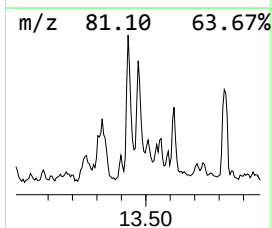
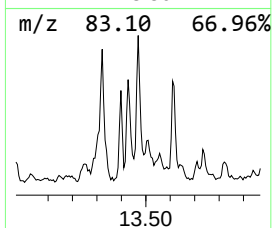
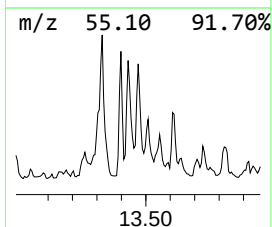
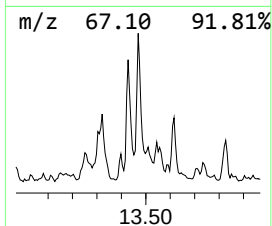
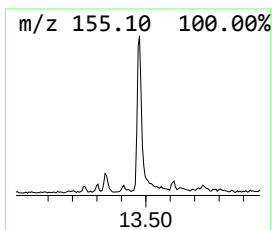
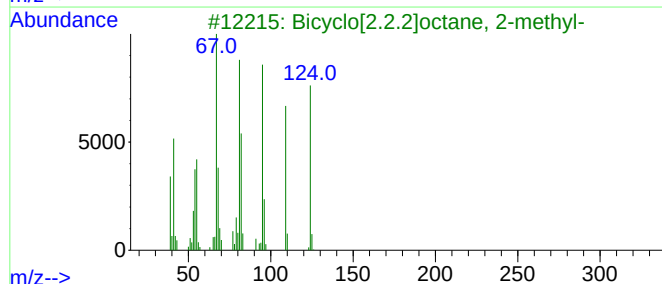
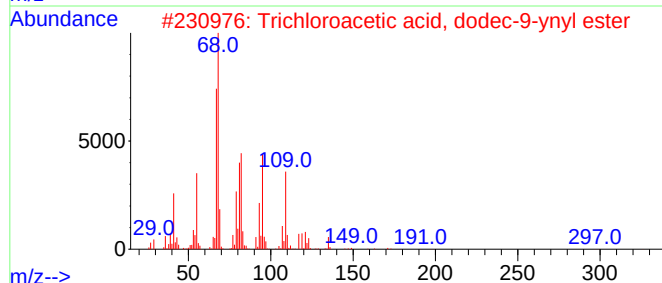
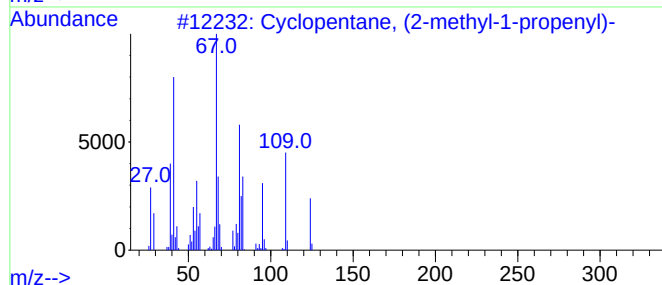
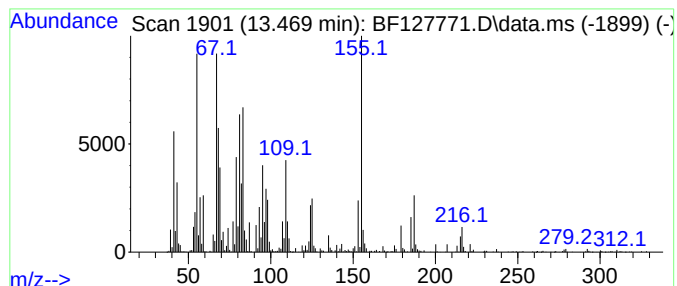
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.469 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.469	27.83 ng	1417050	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, (2-methyl-1-propen...	124	C9H16	053366-57-7	45
2			Trichloroacetic acid, dodec-9-yn...	326	C14H21Cl3O2	1000282-92-3	35
3			Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	35
4			Benzene, 1-fluoro-2-methyl-4-nitro-	155	C7H6FN02	000455-88-9	35
5			2,11-Dodecadiene, 4-chloro-	200	C12H21Cl	1000155-54-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
Data File : BF127771.D
Acq On : 12 Apr 2022 21:29
Operator : CG\JU
Sample : N2365-01 2X
Misc :
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Instrument :
BNA_F
ClientSampleId :
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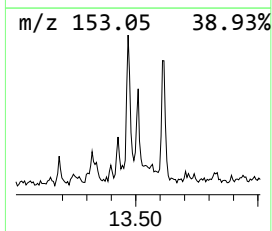
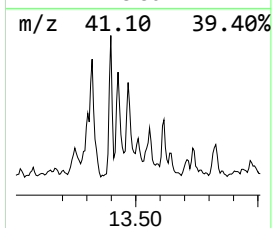
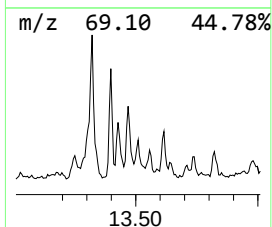
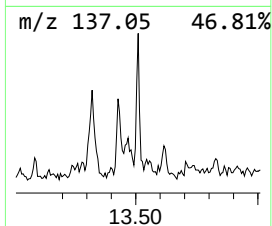
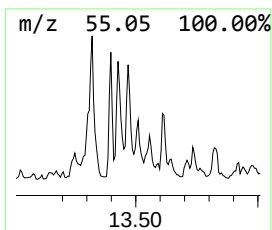
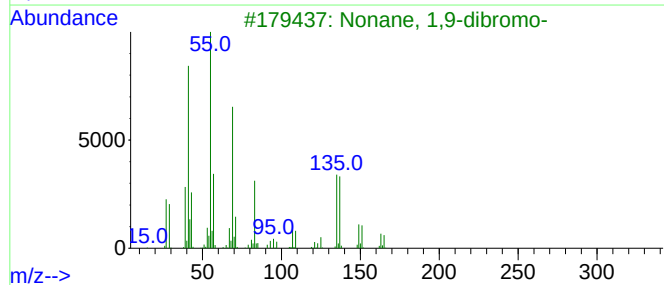
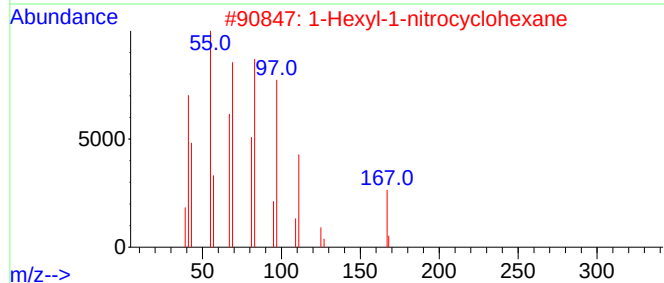
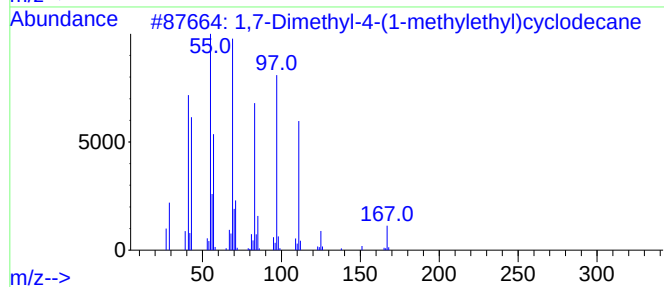
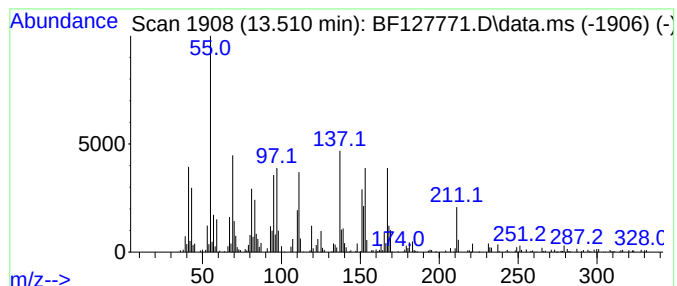
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.510 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.510	12.34 ng	628411	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	14
2			1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	12
3			Nonane, 1,9-dibromo-	284	C9H18Br2	004549-33-1	9
4			10-Methyldodec-2-en-4-olide	210	C13H22O2	1000370-41-0	9
5			9-Tricosene, (Z)-	322	C23H46	027519-02-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
Data File : BF127771.D
Acq On : 12 Apr 2022 21:29
Operator : CG\JU
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Misc :
ALS Vial : 20 Sample Multiplier: 1

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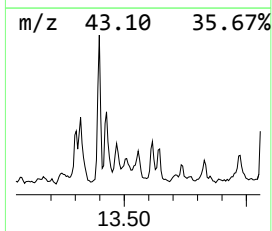
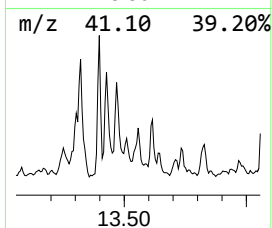
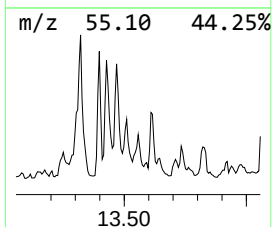
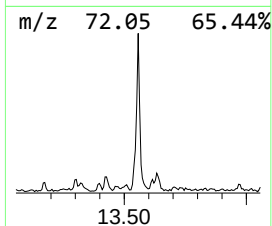
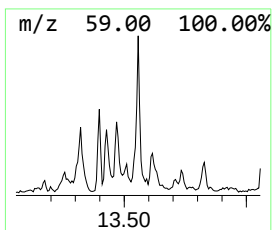
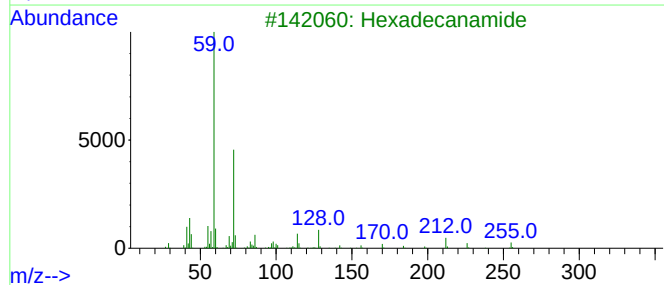
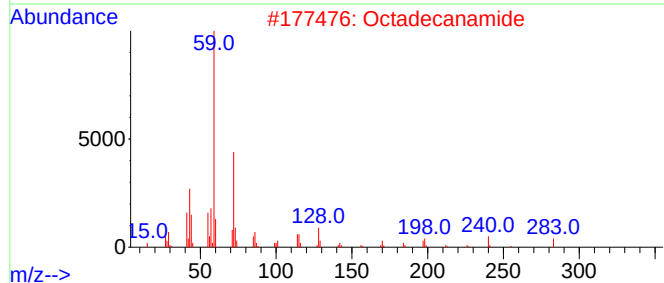
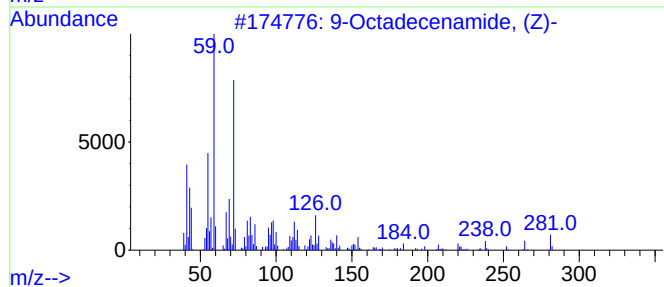
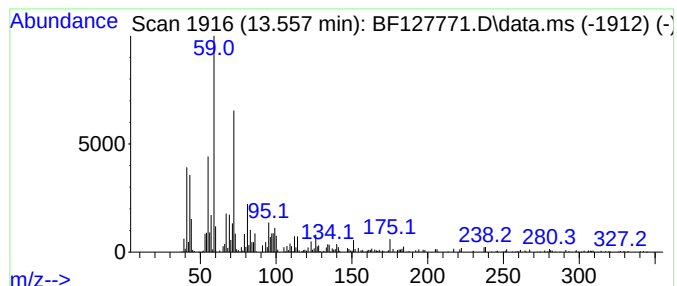
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.557	14.88 ng	757512	Chrysene-d12	14.139

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94	
2	Octadecanamide	283	C18H37NO	000124-26-5	64	
3	Hexadecanamide	255	C16H33NO	000629-54-9	64	
4	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	64	
5	Nonanamide	157	C9H19NO	001120-07-6	52	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
Data File : BF127771.D
Acq On : 12 Apr 2022 21:29
Operator : CG\JU
Sample : N2365-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

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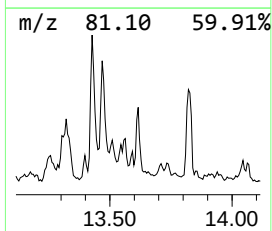
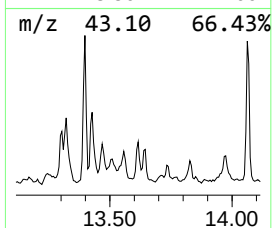
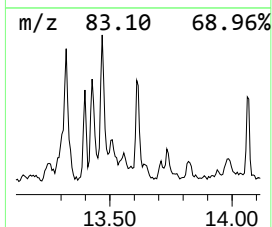
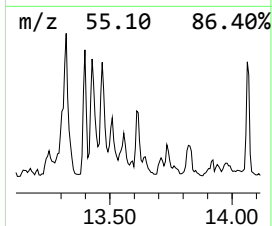
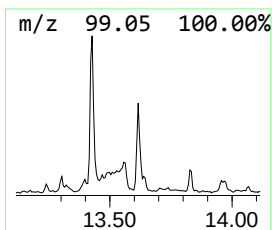
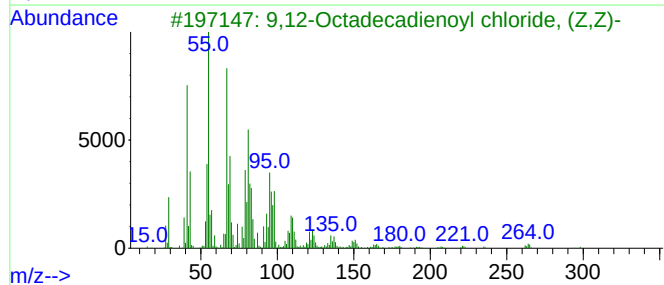
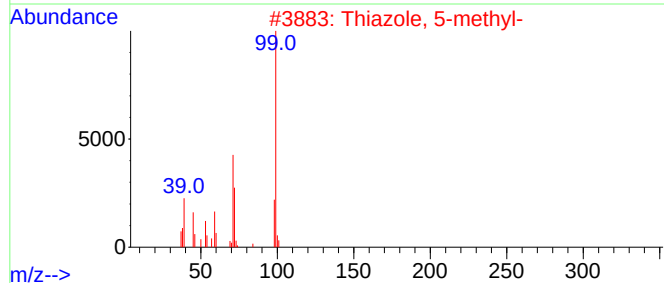
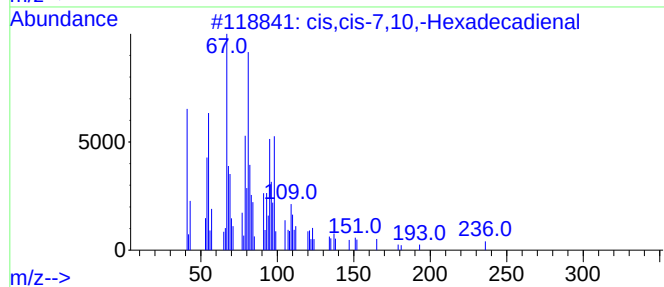
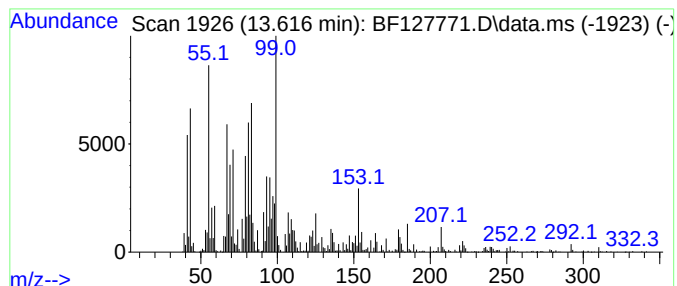
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown13.616 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.616	15.89 ng	809033	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis,cis-7,10,-Hexadecadienal	236	C16H28O	056829-23-3	47
2			Thiazole, 5-methyl-	99	C4H5NS	003581-89-3	38
3			9,12-Octadecadienoyl chloride, (...	298	C18H31ClO	007459-33-8	25
4			(Z)-2-pentylcyclopentanone oxime	169	C10H19NO	1000441-61-3	25
5			Hexanethioic acid, S-decyl ester	272	C16H32OS	002432-81-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
Data File : BF127771.D
Acq On : 12 Apr 2022 21:29
Operator : CG\JU
Sample : N2365-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-04-041122

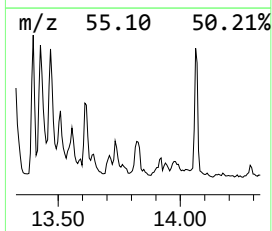
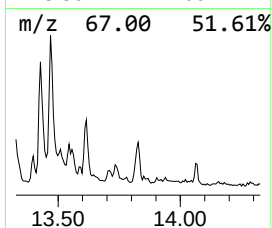
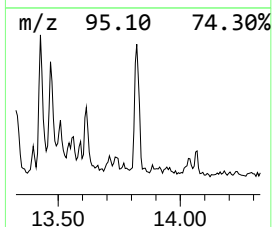
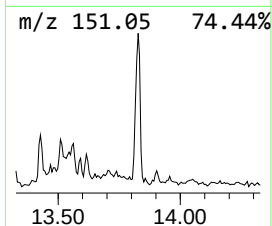
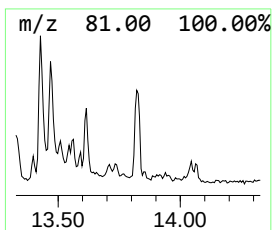
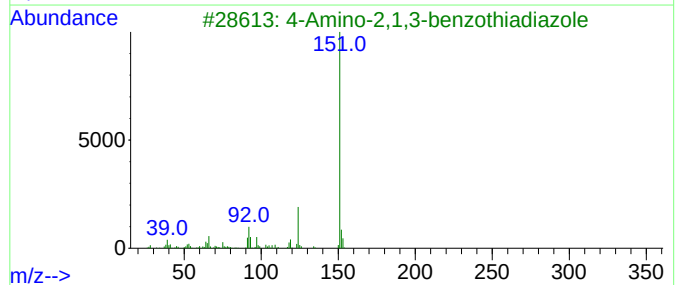
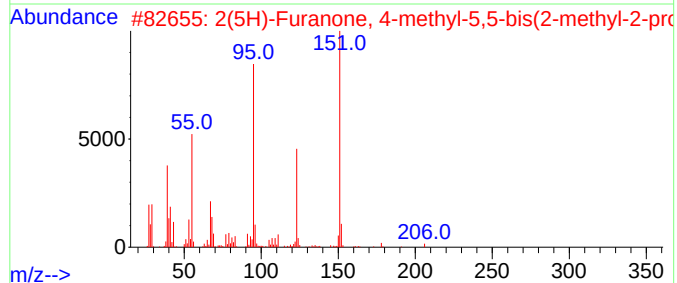
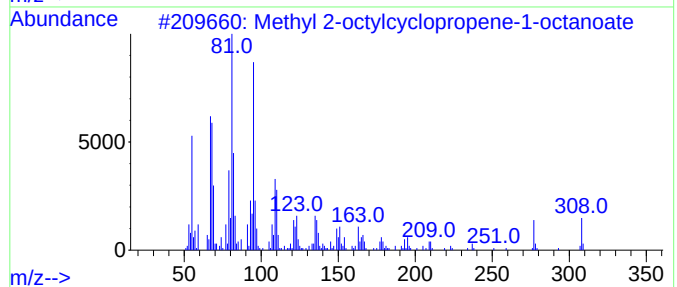
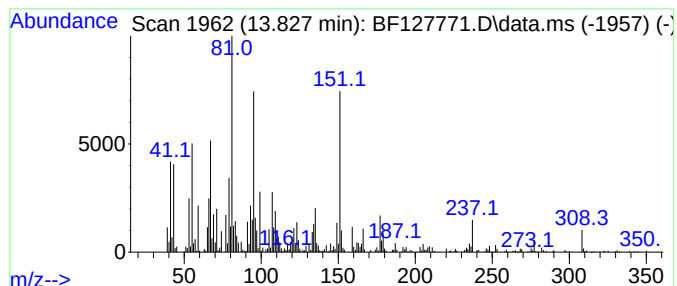
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown13.827 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	13.14 ng	669209	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 2-octylcyclopropene-1-oct...	308	C20H36O2	003220-60-8	43
2			2(5H)-Furanone, 4-methyl-5,5-bis...	206	C13H18O2	099202-98-9	42
3			4-Amino-2,1,3-benzothiadiazole	151	C6H5N3S	000767-64-6	25
4			4-Hydroxybenzoxazolone	151	C7H5NO3	028955-70-6	25
5			RMDI, Cis,trans-	262	C15H22N2O2	017901-48-3	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
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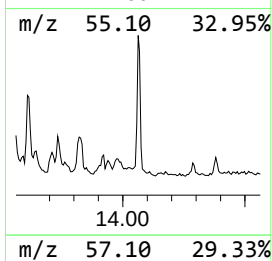
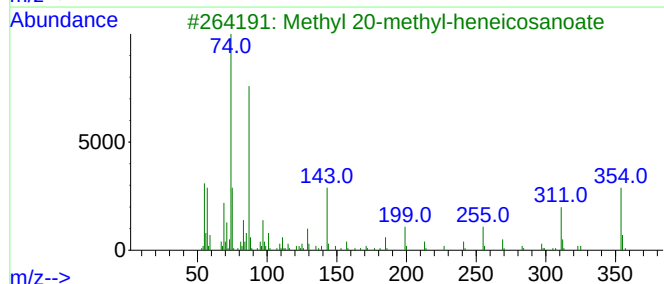
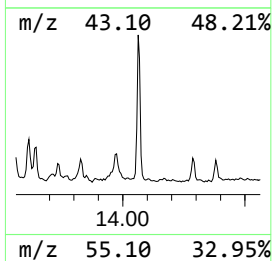
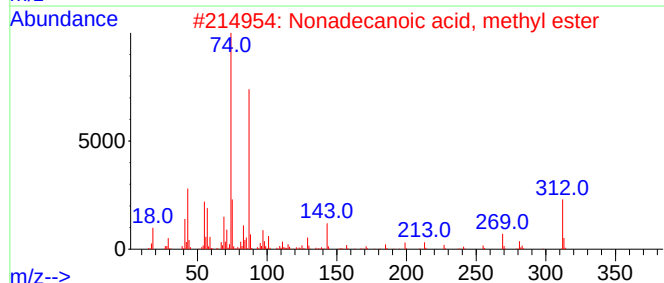
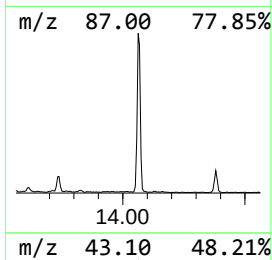
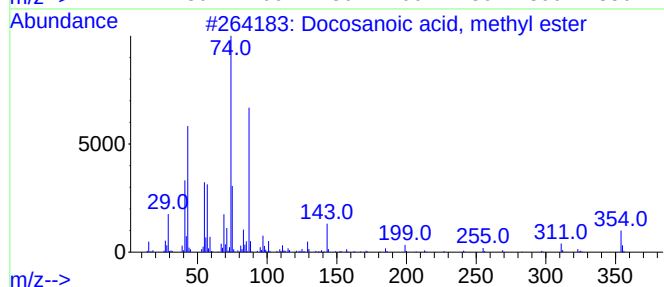
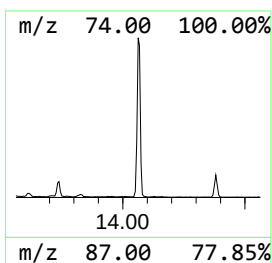
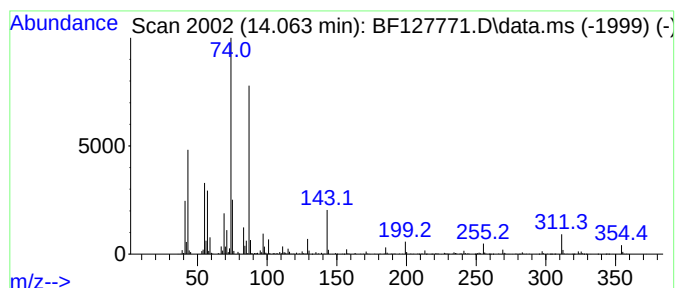
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Docosanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.063	24.94 ng	1270300	Chrysene-d12		14.139	
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	96
3	Methyl 20-methyl-heneicosanoate		354	C23H46O2	1000336-47-4	95
4	Eicosanoic acid, methyl ester		326	C21H42O2	001120-28-1	90
5	Methyl stearate		298	C19H38O2	000112-61-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
Data File : BF127771.D
Acq On : 12 Apr 2022 21:29
Operator : CG\JU
Sample : N2365-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-04-041122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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...	11.892	452.0	ng	19235000	4	11.486	851157	20.0
n-Hexadecanoic ...	12.039	59.9	ng	2550860	4	11.486	851157	20.0
9,12-Octadecadi...	12.633	1393.6	ng	59309400	4	11.486	851157	20.0
cis-13-Eicoseno...	13.322	41.4	ng	2109620	5	14.139	1018510	20.0
Eicosanoic acid...	13.398	29.7	ng	1514670	5	14.139	1018510	20.0
1,6-Cyclodecadiene	13.427	32.5	ng	1653100	5	14.139	1018510	20.0
unknown13.469	13.469	27.8	ng	1417050	5	14.139	1018510	20.0
unknown13.510	13.510	12.3	ng	628411	5	14.139	1018510	20.0
9-Octadecenamid...	13.557	14.9	ng	757512	5	14.139	1018510	20.0
unknown13.616	13.616	15.9	ng	809033	5	14.139	1018510	20.0
unknown13.827	13.827	13.1	ng	669209	5	14.139	1018510	20.0
Docosanoic acid...	14.063	24.9	ng	1270300	5	14.139	1018510	20.0