

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
 Data File : BF128977.D
 Acq On : 24 Jun 2022 03:22
 Operator : CG\JU
 Sample : N3427-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-04-062122

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-BF060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128977.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.357	519	522	539	rBV	885635	907324	24.86%	6.016%
2	6.381	693	696	706	rBV	920553	905902	24.82%	6.007%
3	6.728	751	755	760	rVB	418692	372596	10.21%	2.471%
4	7.292	847	851	854	rBV	705137	564090	15.45%	3.740%
5	7.322	854	856	859	rVB	123206	89325	2.45%	0.592%
6	7.757	927	930	935	rVB2	33134	36784	1.01%	0.244%
7	7.992	967	970	971	rBV	152934	135424	3.71%	0.898%
8	8.010	971	973	976	rVV	516671	392112	10.74%	2.600%
9	8.069	979	983	986	rVB	47654	45285	1.24%	0.300%
10	8.298	1018	1022	1029	rVB4	27923	49780	1.36%	0.330%
11	8.428	1041	1044	1046	rBV	68947	59454	1.63%	0.394%
12	9.028	1144	1146	1152	rVB2	45889	36521	1.00%	0.242%
13	9.086	1152	1156	1159	rBV	1302350	970715	26.59%	6.437%
14	9.157	1164	1168	1175	rBV6	22640	42028	1.15%	0.279%
15	9.486	1219	1224	1226	rVB5	34429	38917	1.07%	0.258%
16	9.763	1267	1271	1275	rVB	529466	405881	11.12%	2.691%
17	10.557	1402	1406	1415	rBV	491595	468666	12.84%	3.108%
18	11.251	1520	1524	1526	rBV	482340	405655	11.11%	2.690%
19	11.645	1587	1591	1594	rBV	786131	608580	16.67%	4.035%
20	11.863	1625	1628	1634	rVB5	25793	48278	1.32%	0.320%
21	12.298	1699	1702	1704	rBV	35713	38705	1.06%	0.257%
22	12.339	1704	1709	1710	rVV	3388625	3650121	100.00%	24.203%
23	12.357	1710	1712	1718	rVV	2747083	2276144	62.36%	15.093%
24	12.439	1722	1726	1728	rVV	498480	437391	11.98%	2.900%
25	12.463	1728	1730	1734	rVB	94704	79135	2.17%	0.525%
26	12.692	1764	1769	1777	rBV	126106	215610	5.91%	1.430%
27	12.839	1790	1794	1797	rBV	1127182	949134	26.00%	6.294%
28	13.163	1847	1849	1851	rVB	59347	43943	1.20%	0.291%
29	13.898	1970	1974	1976	rBV2	389865	393976	10.79%	2.612%
30	13.992	1987	1990	1994	rVB2	127606	127361	3.49%	0.845%
31	15.339	2215	2219	2223	rVB	226172	286330	7.84%	1.899%

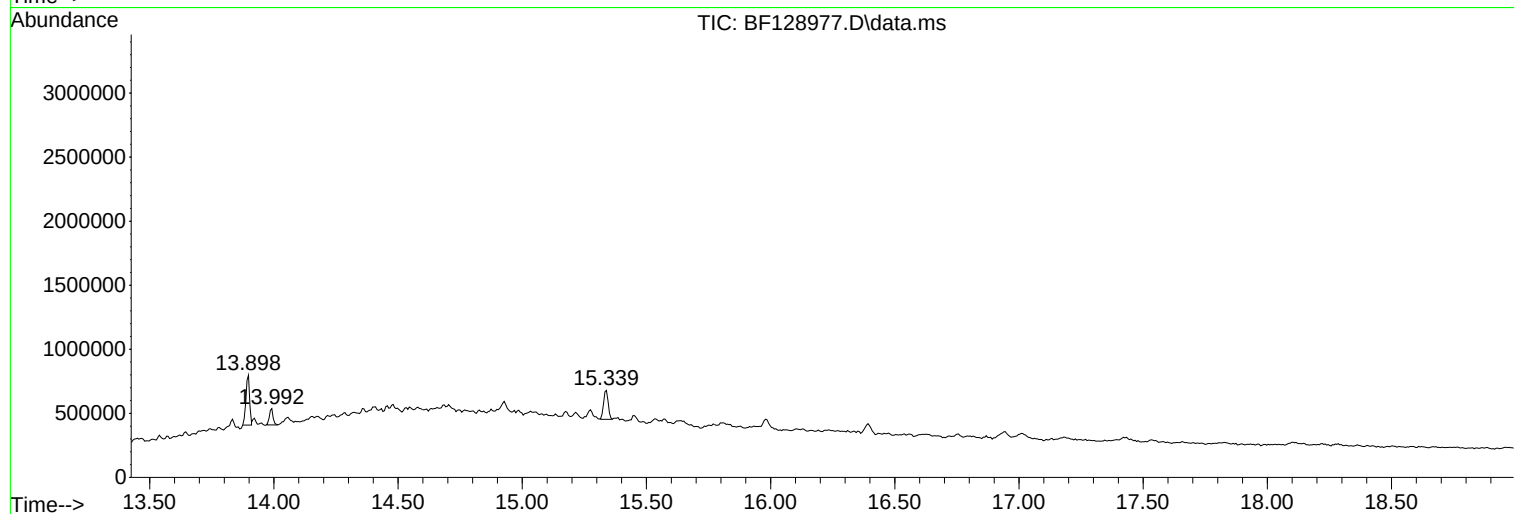
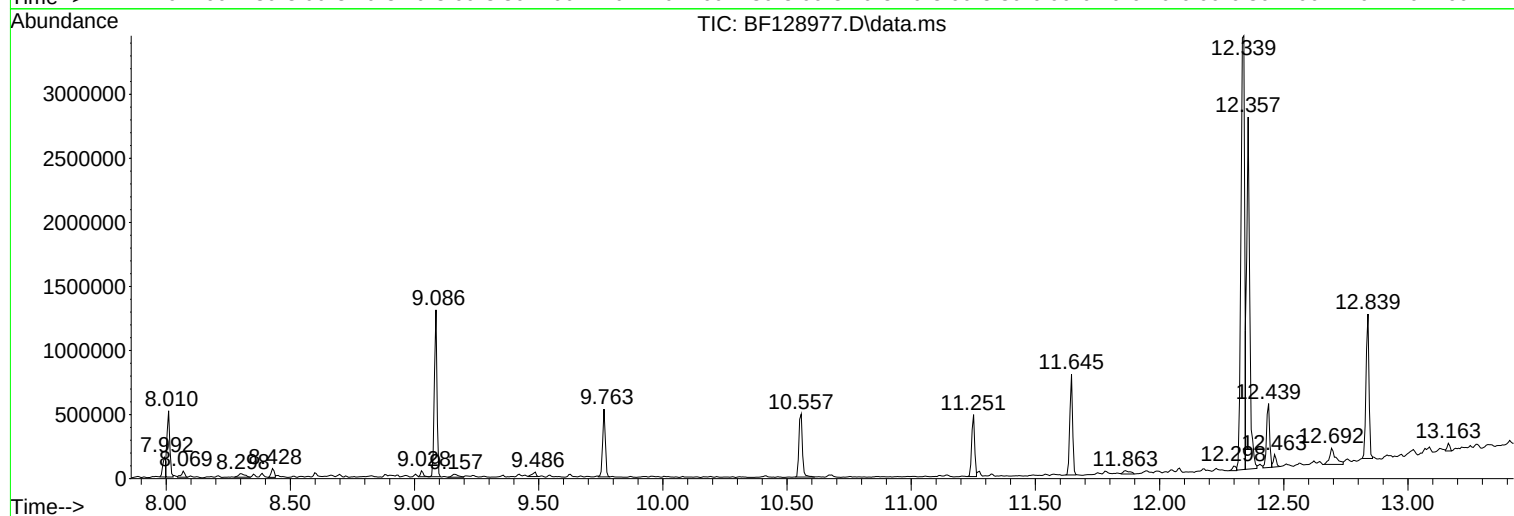
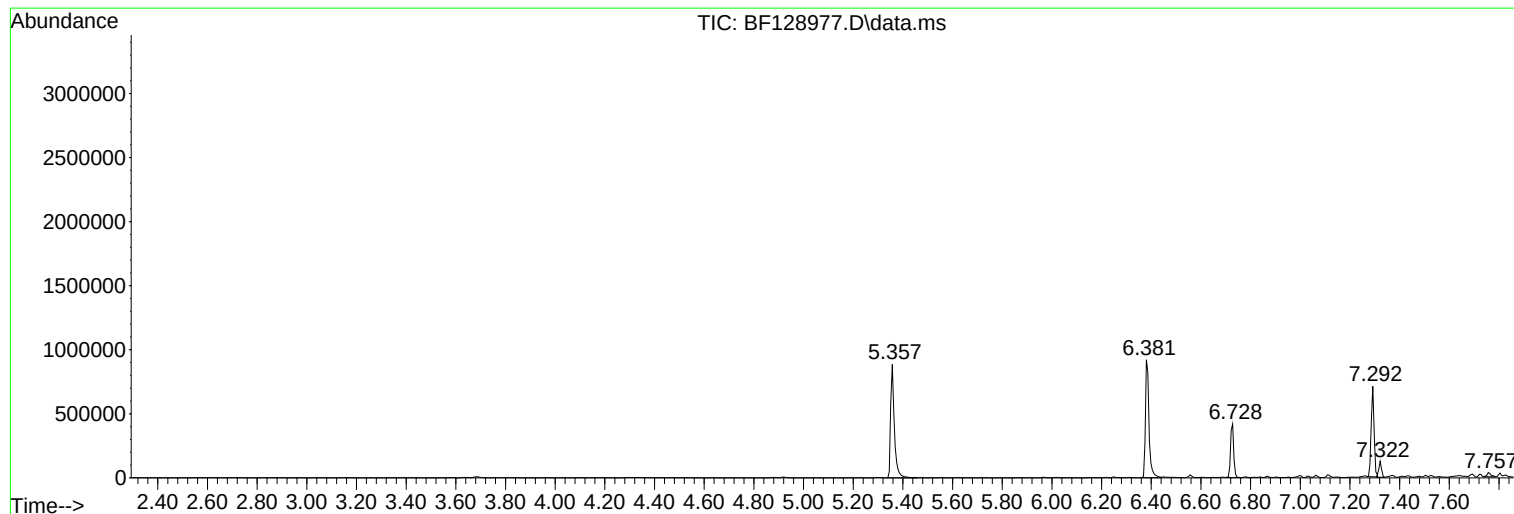
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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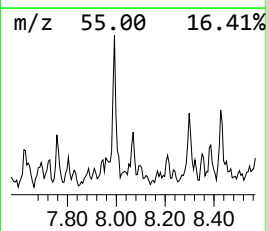
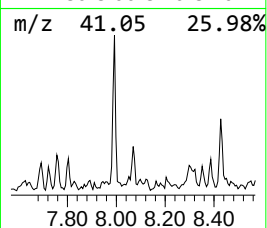
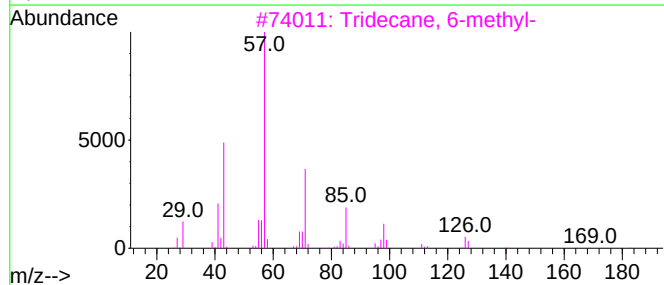
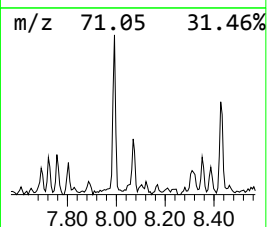
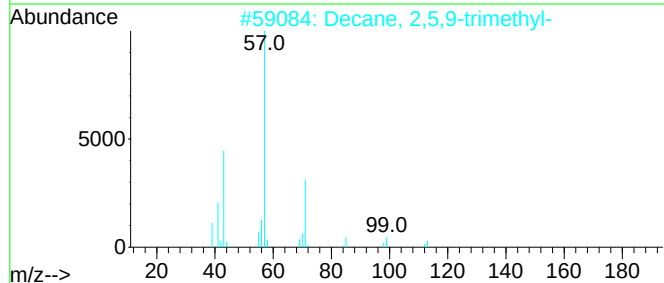
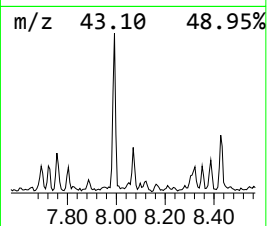
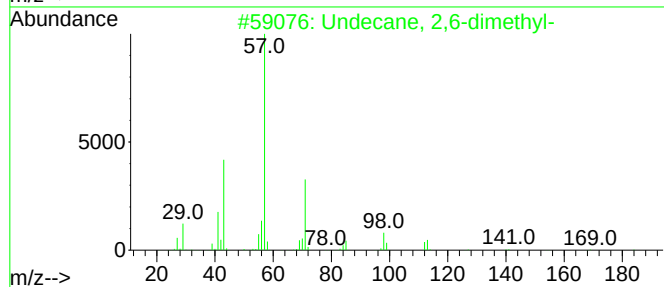
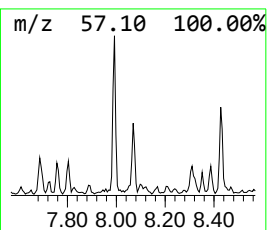
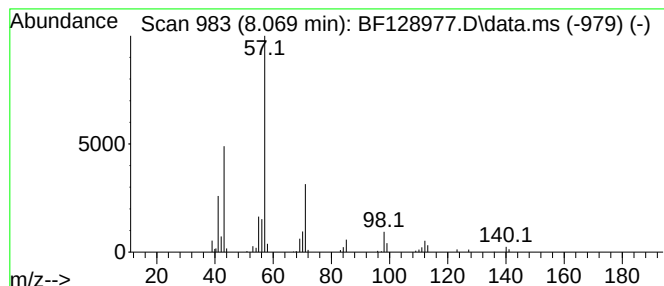
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Undecane, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	2.31 ng	45285	Naphthalene-d8	8.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	72
2			Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	64
3			Tridecane, 6-methyl-	198	C14H30	013287-21-3	64
4			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	59
5			Nonane, 4-methyl-	142	C10H22	017301-94-9	59



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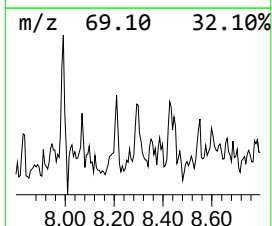
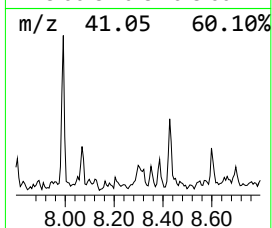
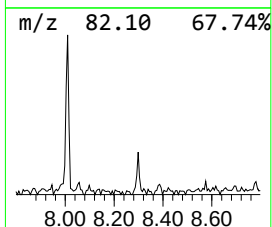
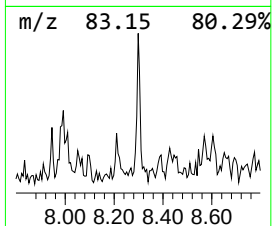
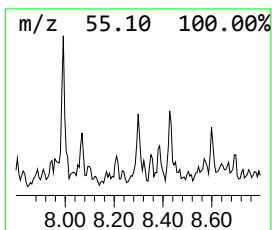
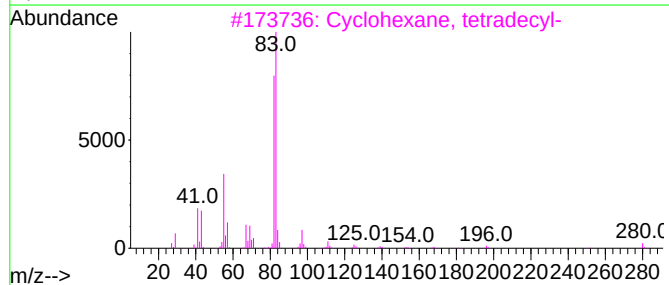
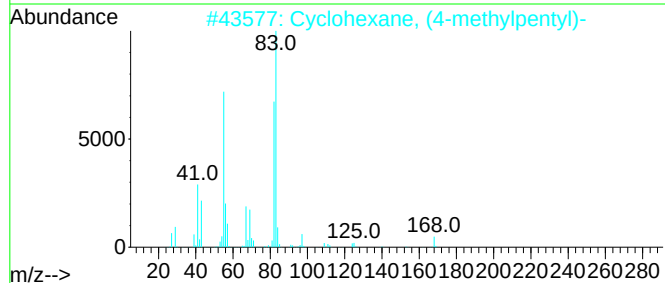
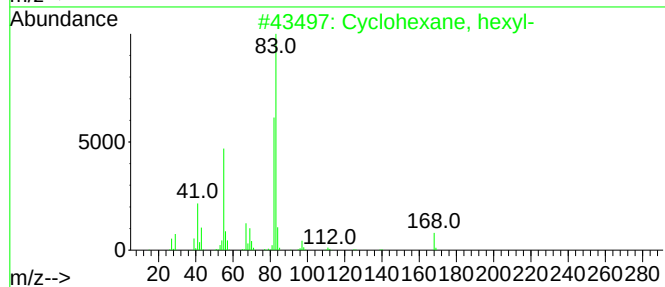
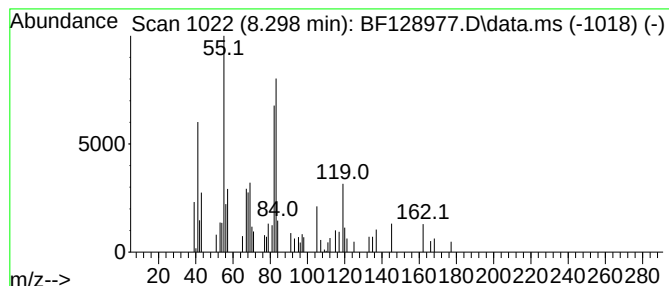
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown8.298 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.298	2.54 ng	49780	Naphthalene-d8	8.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, hexyl-	168	C12H24	004292-75-5	49
2			Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	43
3			Cyclohexane, tetradecyl-	280	C20H40	001795-18-2	43
4			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	43
5			Cyclohexane, nonadecyl-	350	C25H50	022349-03-7	43



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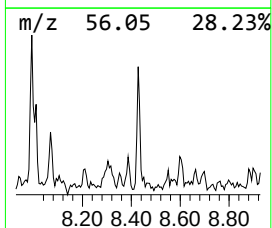
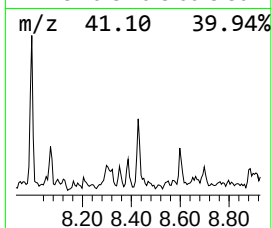
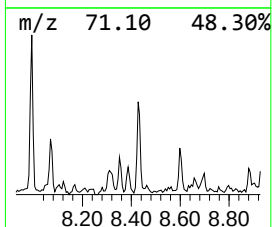
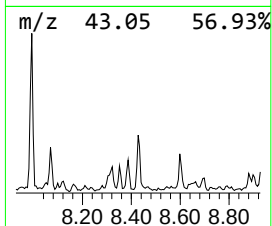
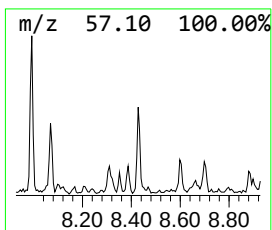
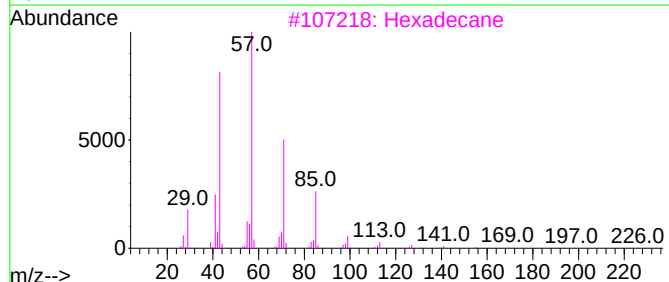
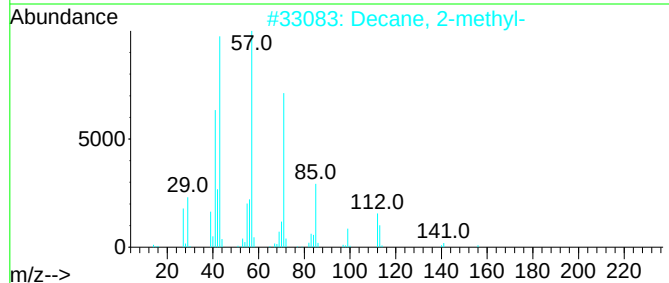
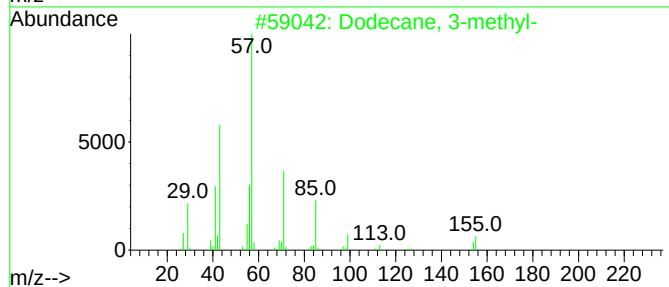
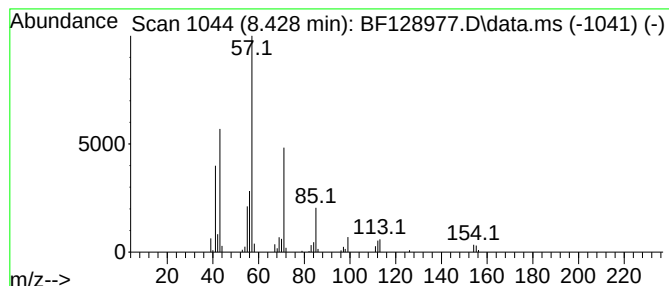
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Dodecane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.428	3.03 ng	59454	Naphthalene-d8	8.010

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane, 3-methyl-	184	C13H28	017312-57-1	86
2		Decane, 2-methyl-	156	C11H24	006975-98-0	64
3		Hexadecane	226	C16H34	000544-76-3	64
4		Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	64
5		Decane, 3-methyl-	156	C11H24	013151-34-3	64



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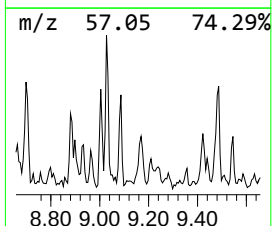
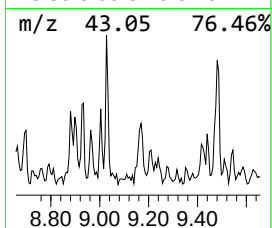
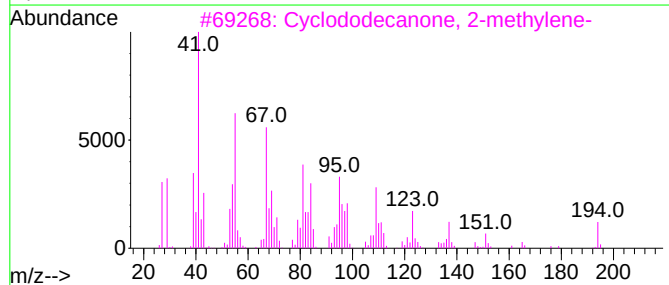
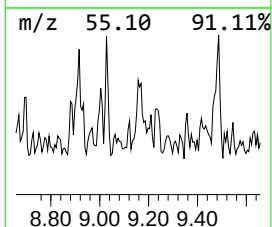
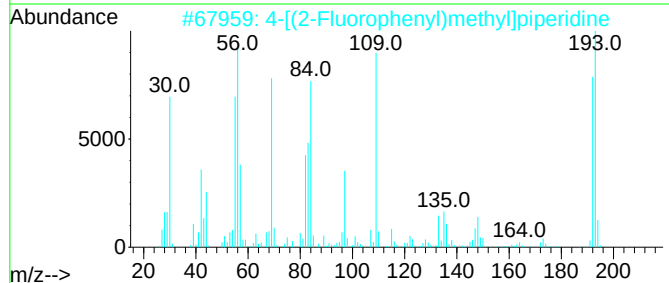
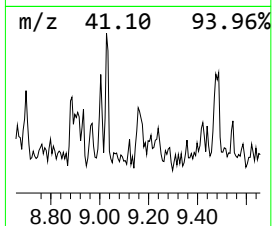
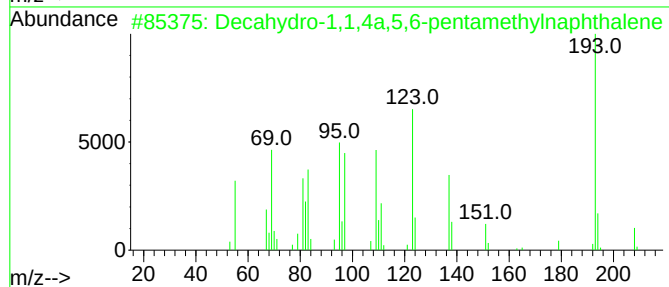
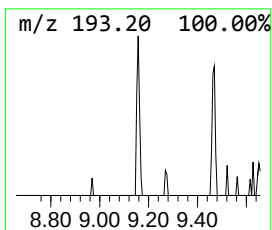
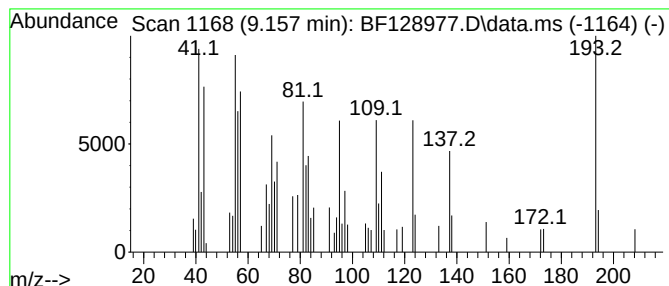
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.157	2.07 ng	42028	Acenaphthene-d10	9.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	93
2	4-[(2-Fluorophenyl)methyl]piperi...	193	C12H16FN	194288-97-6	50
3	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	43
4	2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	007056-56-6	30
5	4-[(4-Fluorophenyl)methyl]piperi...	193	C12H16FN	092822-02-1	30



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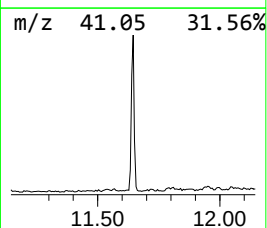
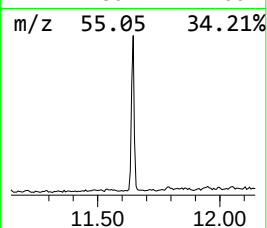
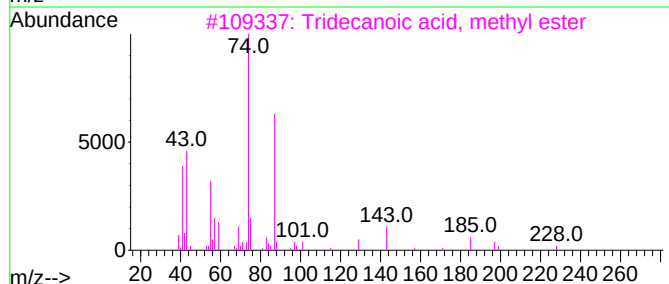
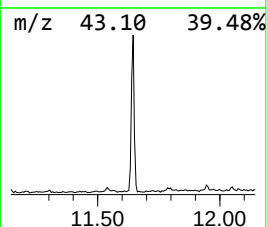
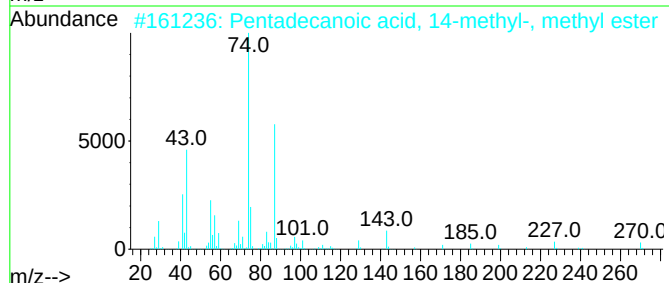
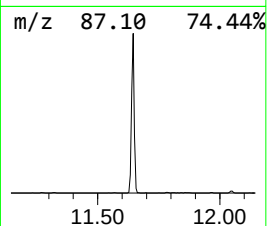
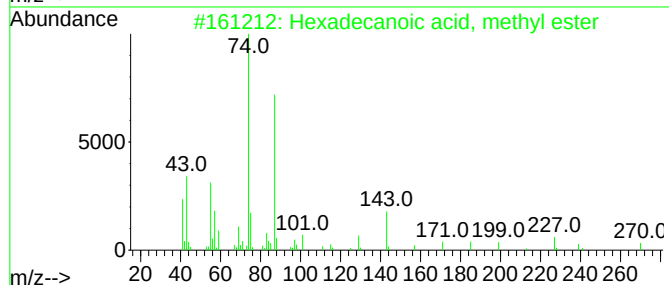
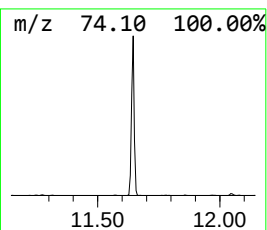
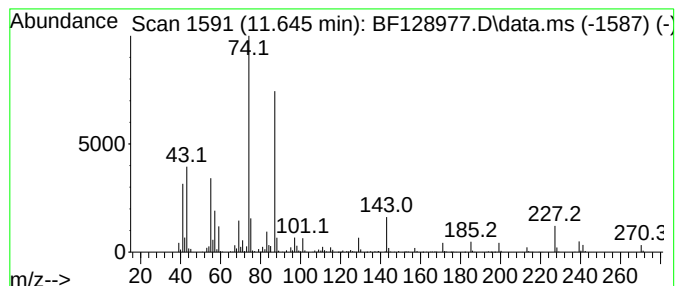
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Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.645	30.00 ng	608580	Phenanthrene-d10	11.251

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	95
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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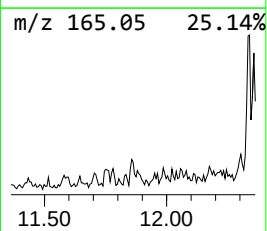
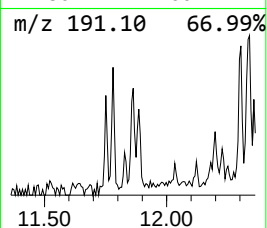
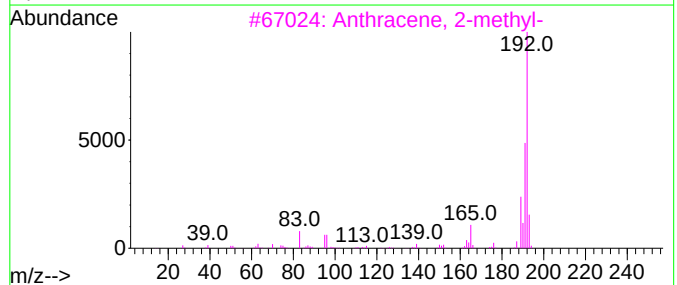
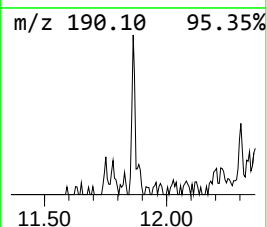
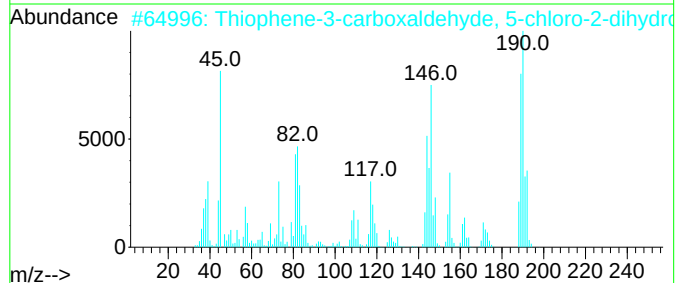
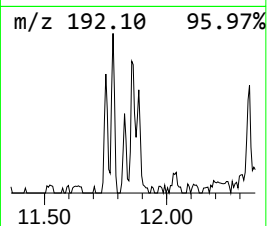
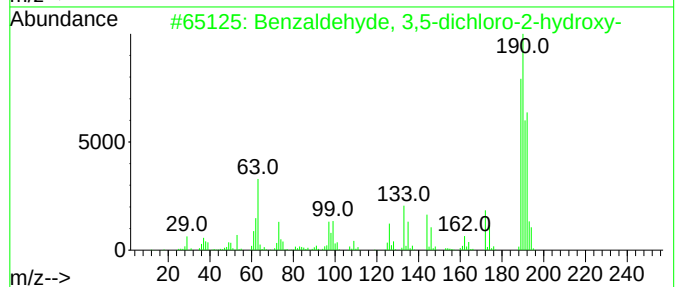
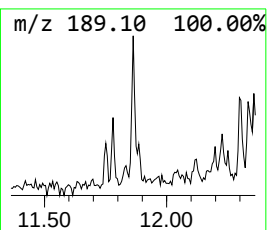
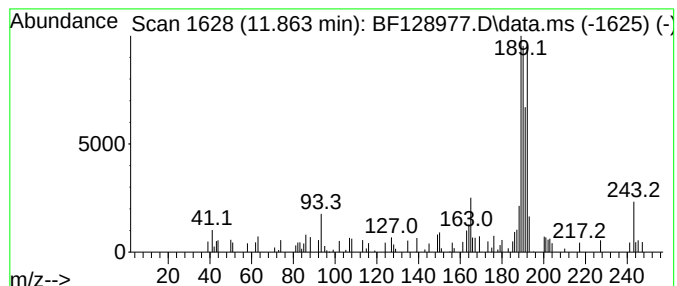
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BNA_F
ClientSampleId :
TR-04-062122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzaldehyde, 3,5-dichloro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.863	2.38 ng	48278	Phenanthrene-d10	11.251	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	49
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	42
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38
5	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128977.D
Acq On : 24 Jun 2022 03:22
Operator : CG\JU
Sample : N3427-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

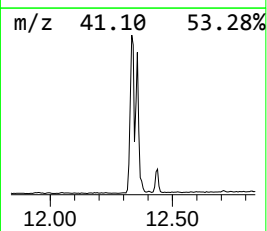
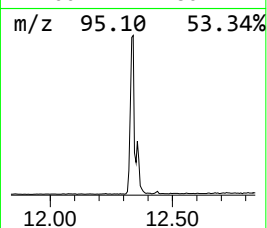
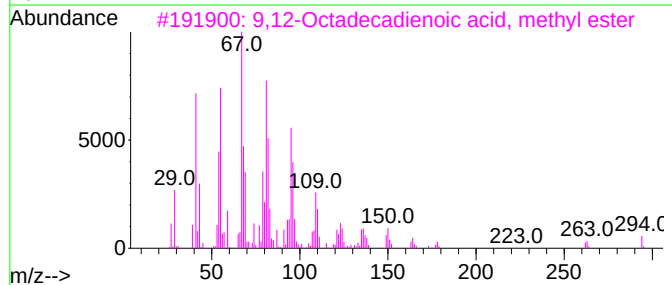
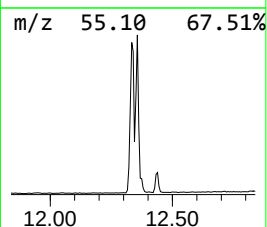
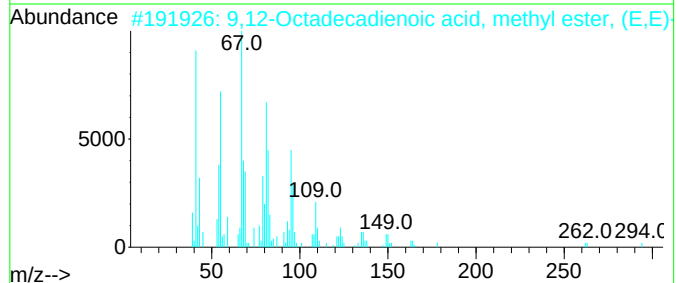
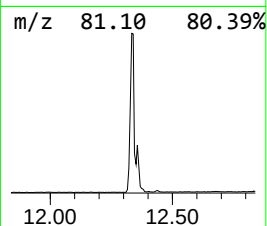
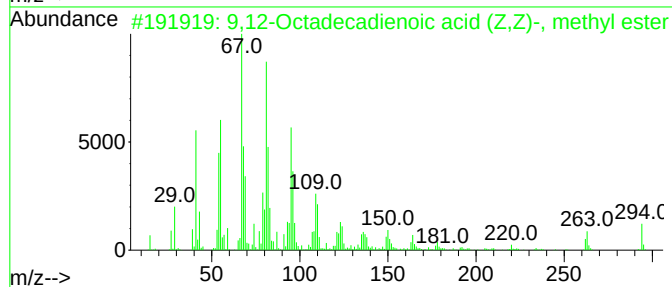
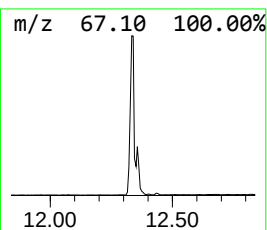
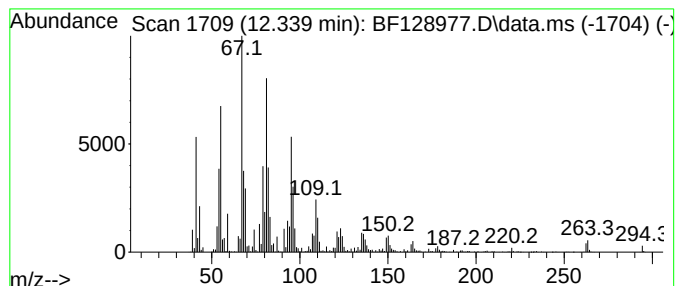
Instrument :
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ClientSampleId :
TR-04-062122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.339	179.96 ng	3650120	Phenanthrene-d10	11.251
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		9,12-Octadecadienoic acid (Z,Z)-...	294 C19H34O2	000112-63-0 99
2		9,12-Octadecadienoic acid, methy...	294 C19H34O2	002566-97-4 99
3		9,12-Octadecadienoic acid, methy...	294 C19H34O2	002462-85-3 99
4		9,15-Octadecadienoic acid, methy...	294 C19H34O2	017309-05-6 99
5		8,11-Octadecadienoic acid, methy...	294 C19H34O2	056599-58-7 98



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128977.D
Acq On : 24 Jun 2022 03:22
Operator : CG\JU
Sample : N3427-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
TR-04-062122

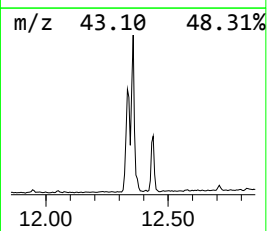
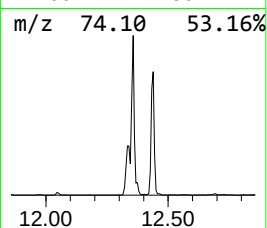
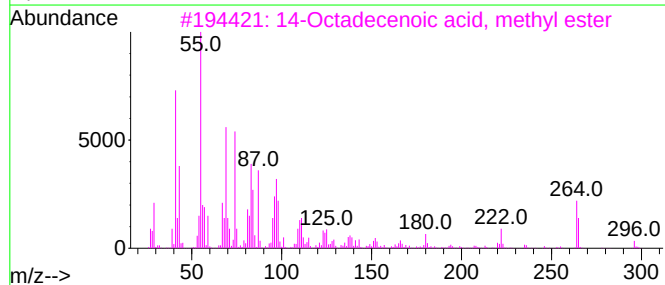
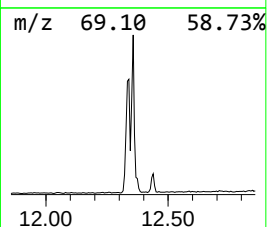
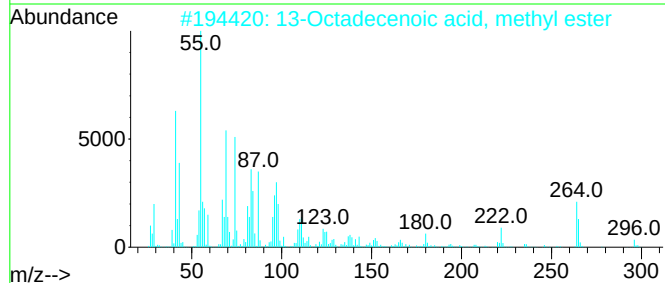
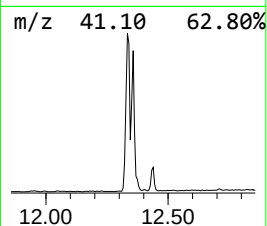
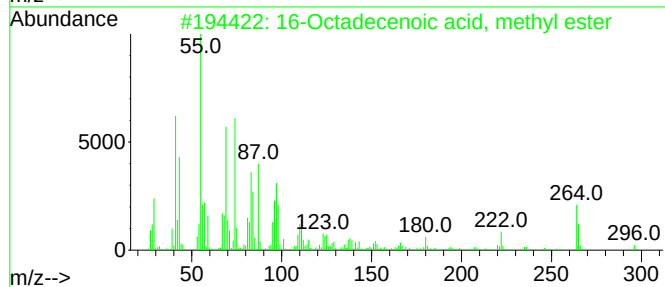
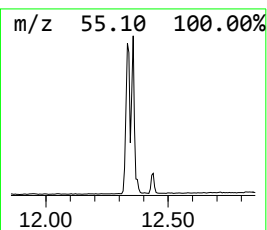
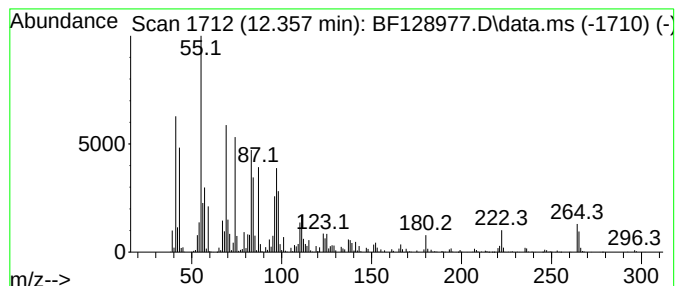
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 16-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	112.22 ng	2276140	Phenanthrene-d10	11.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	96
2			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	96
3			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	95
4			(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	93
5			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128977.D
Acq On : 24 Jun 2022 03:22
Operator : CG\JU
Sample : N3427-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-062122

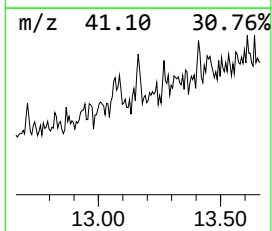
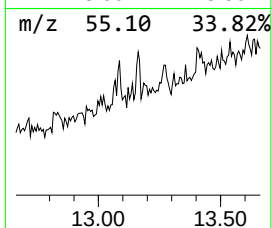
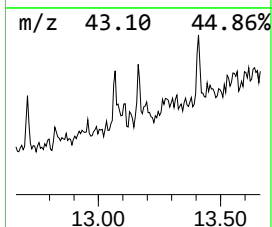
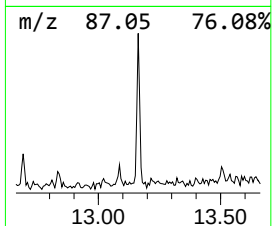
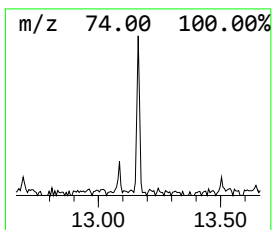
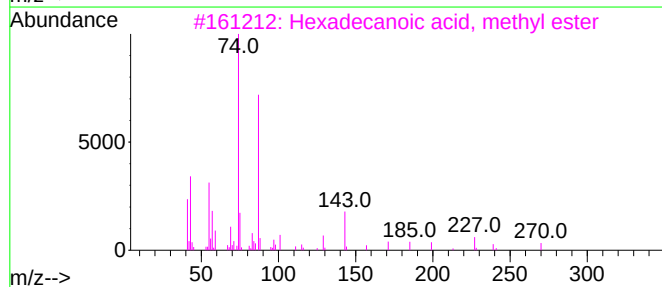
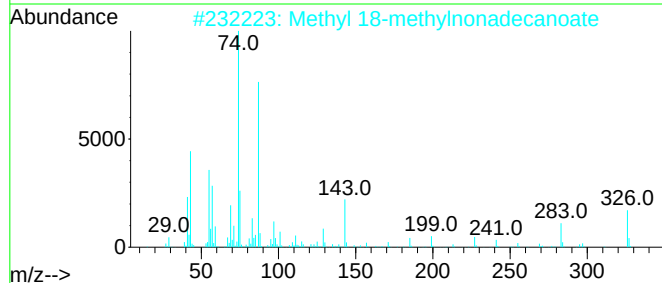
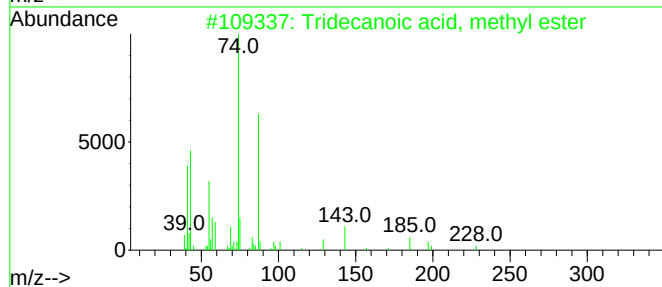
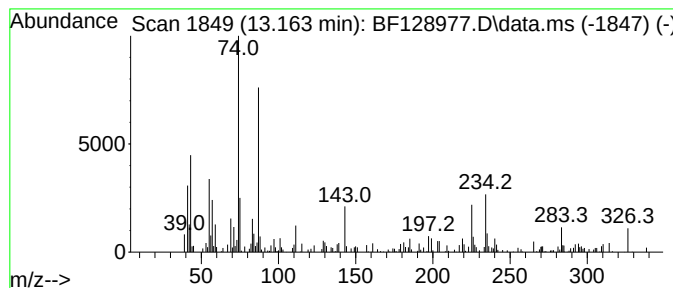
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tridecanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	2.23 ng	43943	Chrysene-d12	13.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
2			Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	89
3			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
4			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86
5			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128977.D
Acq On : 24 Jun 2022 03:22
Operator : CG\JU
Sample : N3427-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-062122

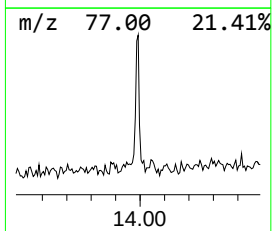
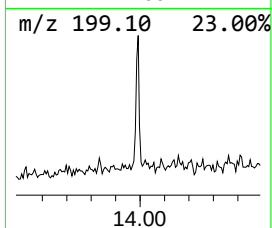
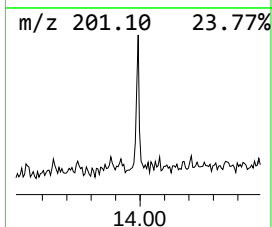
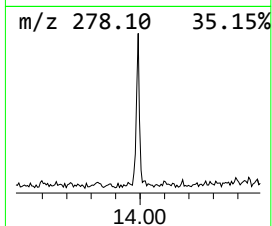
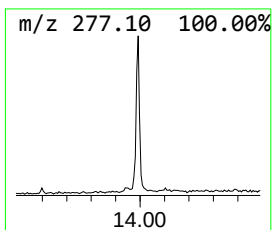
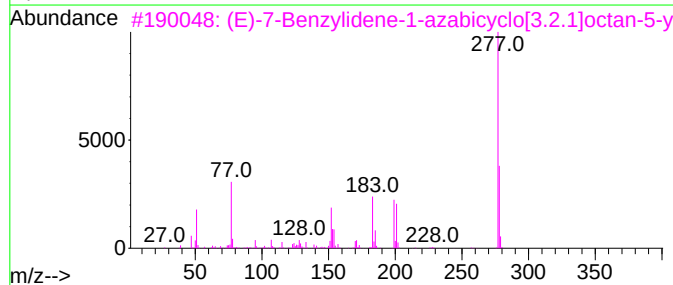
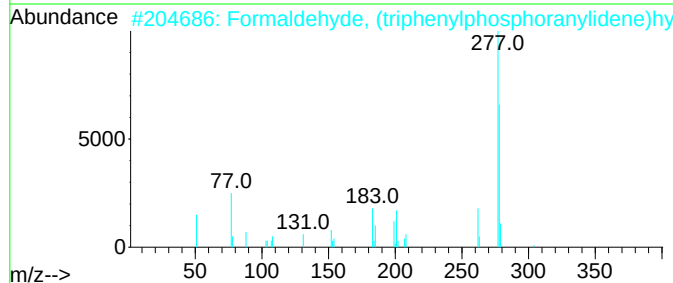
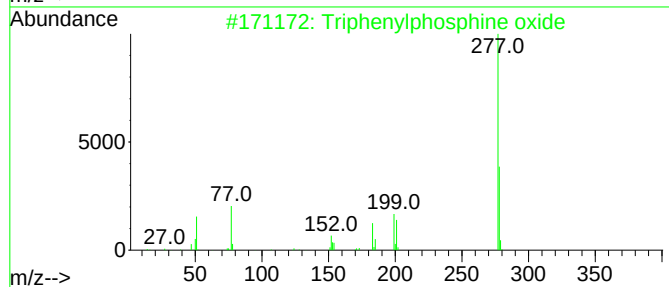
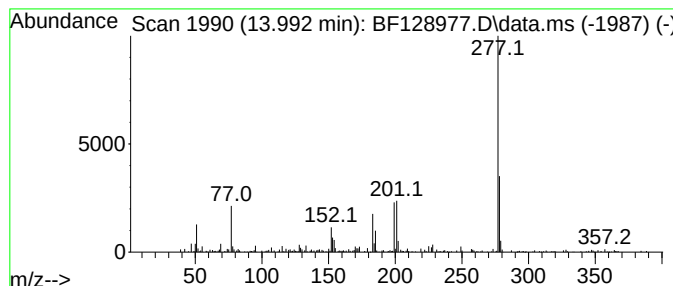
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	6.47 ng	127361	Chrysene-d12	13.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	47
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128977.D
Acq On : 24 Jun 2022 03:22
Operator : CG\JU
Sample : N3427-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-062122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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
Undecane, 2,6-d...	8.069	2.3	ng	45285	2	8.010	392112	20.0
unknown8.298	8.298	2.5	ng	49780	2	8.010	392112	20.0
Dodecane, 3-met...	8.428	3.0	ng	59454	2	8.010	392112	20.0
Decahydro-1,1,4...	9.157	2.1	ng	42028	3	9.763	405881	20.0
Hexadecanoic ac...	11.645	30.0	ng	608580	4	11.251	405655	20.0
Benzaldehyde, 3...	11.863	2.4	ng	48278	4	11.251	405655	20.0
9,12-Octadecadi...	12.339	180.0	ng	3650120	4	11.251	405655	20.0
16-Octadecenoic...	12.357	112.2	ng	2276140	4	11.251	405655	20.0
Tridecanoic aci...	13.163	2.2	ng	43943	5	13.898	393976	20.0
Triphenylphosph...	13.992	6.5	ng	127361	5	13.898	393976	20.0