

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121220\
 Data File : BF122676.D
 Acq On : 12 Dec 2020 14:04
 Operator : JU/CG
 Sample : L5042-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 KENS-B6-121020-0-6

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-BF120520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122676.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.463	568	574	577	rBV	3650433	3684471	44.80%	8.175%
2	6.475	740	746	763	rBV	3369408	4082987	49.64%	9.059%
3	6.675	777	780	791	rBV	72452	101991	1.24%	0.226%
4	6.834	804	807	811	rBV	964525	819212	9.96%	1.818%
5	7.398	898	903	906	rBV	2315800	2535318	30.83%	5.625%
6	8.122	1021	1026	1029	rBV	1122953	1075815	13.08%	2.387%
7	9.198	1203	1209	1212	rBV	4732787	4599103	55.92%	10.204%
8	9.586	1271	1275	1279	rBV	386015	325793	3.96%	0.723%
9	9.875	1319	1324	1327	rBV	1459702	1262732	15.35%	2.802%
10	10.663	1453	1458	1468	rBV	2721399	2611674	31.75%	5.795%
11	11.357	1572	1576	1580	rBV	1357080	1263422	15.36%	2.803%
12	11.898	1659	1668	1687	rVB	2564871	4831269	58.74%	10.719%
13	12.539	1773	1777	1780	rBV2	265000	394557	4.80%	0.875%
14	12.586	1780	1785	1787	rBV5	167822	272594	3.31%	0.605%
15	12.692	1793	1803	1827	rVB	4405669	8224810	100.00%	18.248%
16	12.951	1841	1847	1850	rBV	4773896	4715127	57.33%	10.461%
17	13.669	1961	1969	1978	rBV	160340	382181	4.65%	0.848%
18	13.827	1992	1996	1998	rVV	102810	146070	1.78%	0.324%
19	13.869	1998	2003	2020	rVV3	336174	821097	9.98%	1.822%
20	13.998	2021	2025	2034	rVB	1311063	1220504	14.84%	2.708%
21	14.392	2086	2092	2099	rVV	137317	272304	3.31%	0.604%
22	15.027	2194	2200	2208	rVB2	98954	178507	2.17%	0.396%
23	15.463	2269	2274	2281	rBV	853378	1134881	13.80%	2.518%
24	16.186	2392	2397	2410	rVB7	48031	115051	1.40%	0.255%

Sum of corrected areas: 45071470

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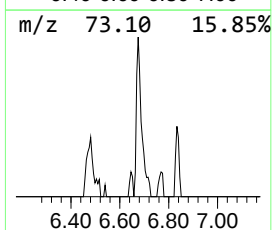
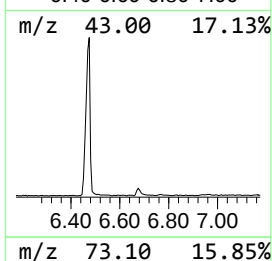
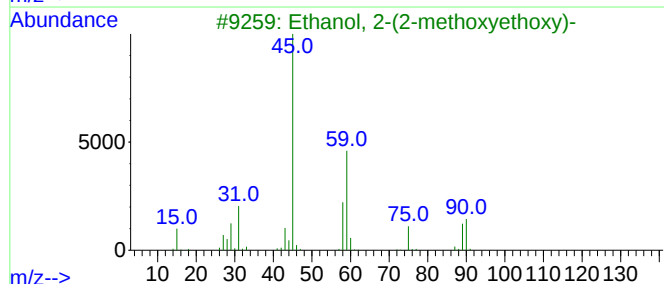
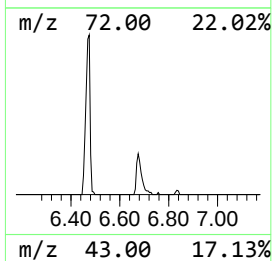
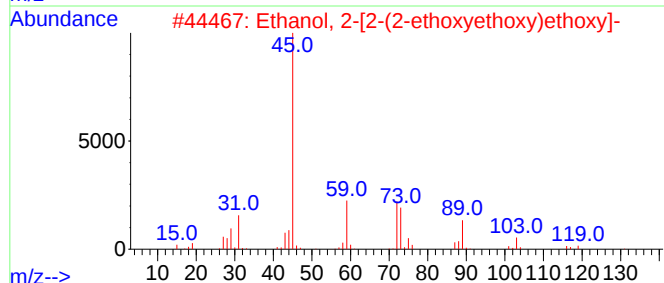
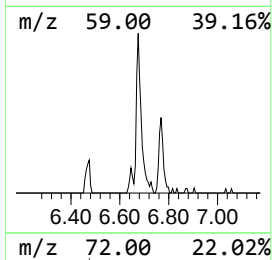
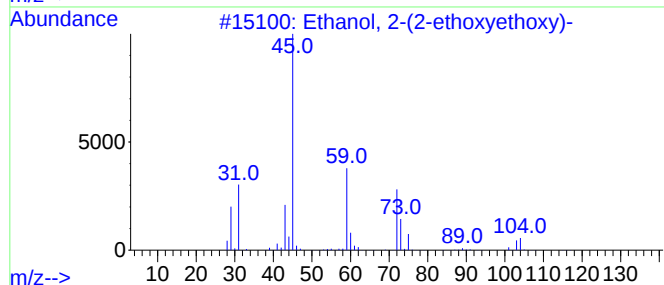
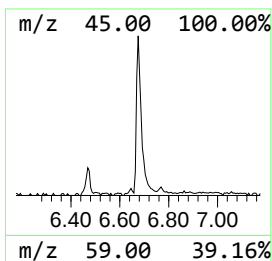
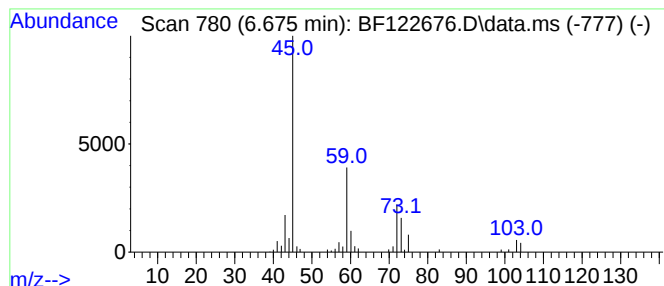
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.675	2.49 ng	101991	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	53
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5			Isoxazolidine	73	C3H7NO	000504-72-3	43



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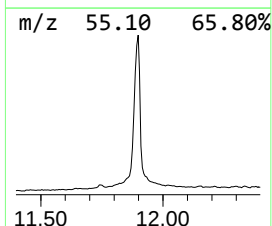
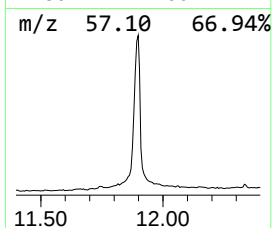
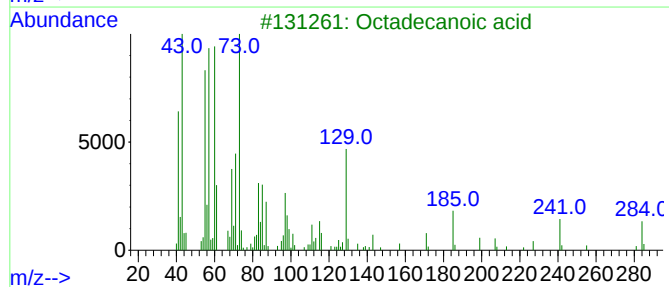
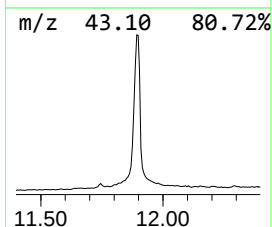
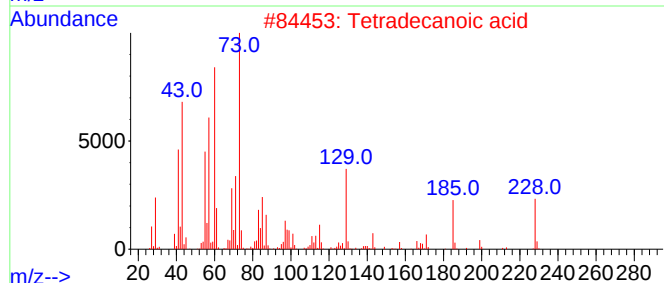
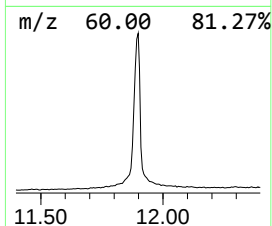
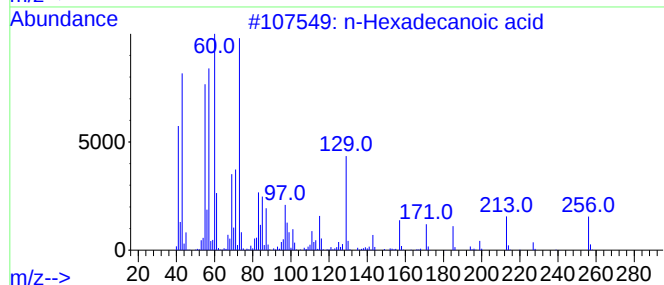
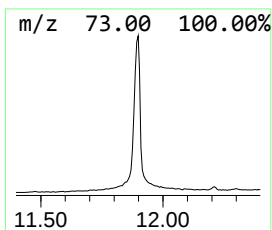
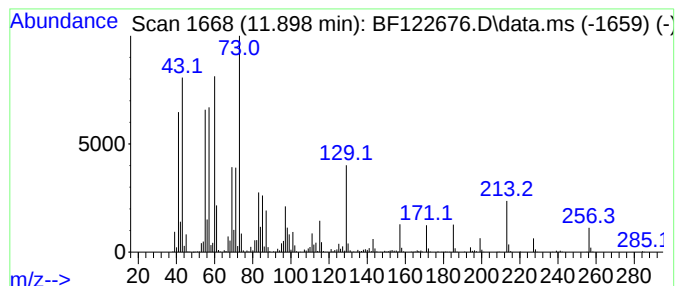
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	76.48 ng	4831270	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			Tridecanoic acid	214	C13H26O2	000638-53-9	81



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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KENS-B6-121020-0-6

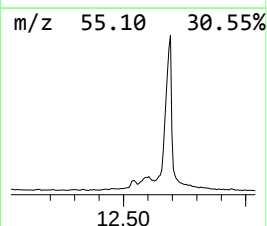
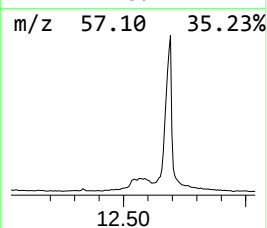
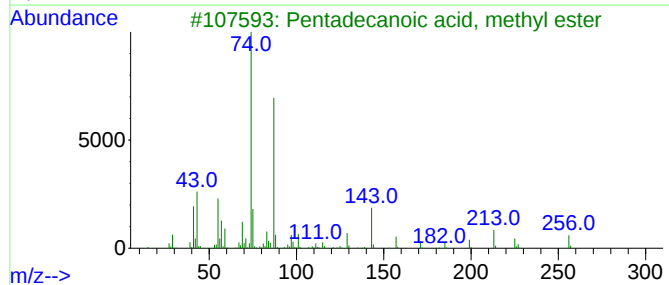
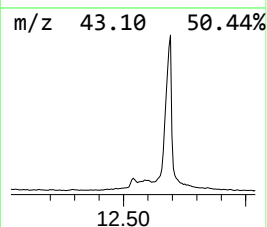
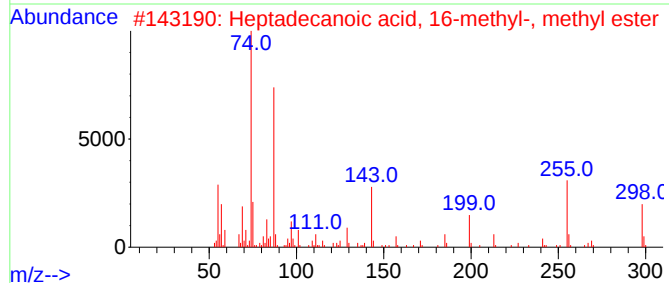
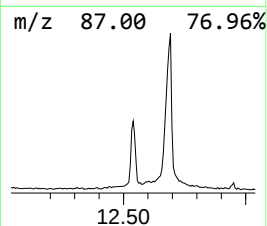
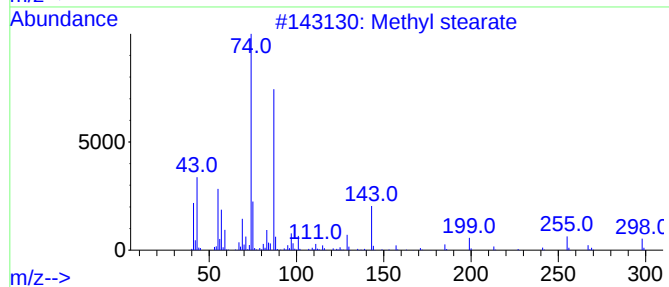
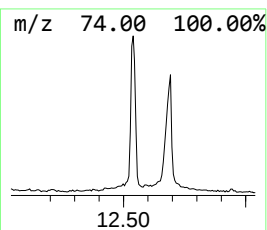
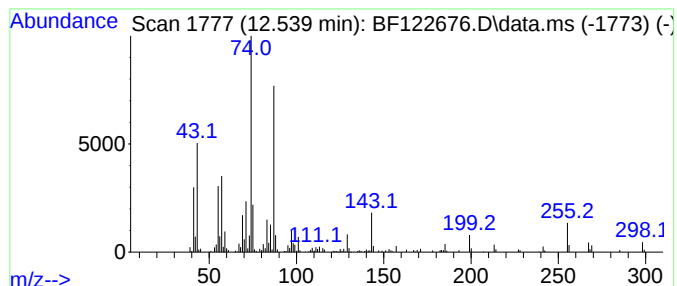
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.539	6.25 ng	394557	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4			Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	80
5			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	76



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Misc :
ALS Vial : 4 Sample Multiplier: 1

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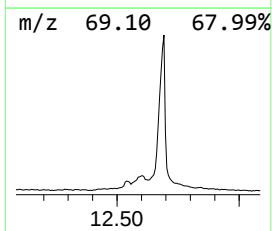
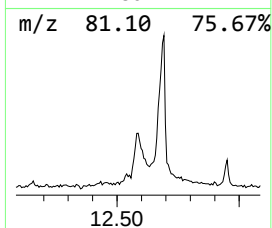
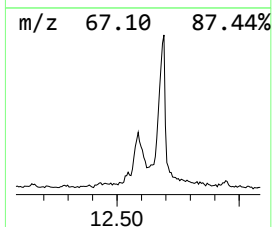
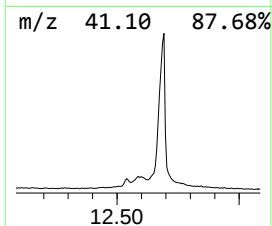
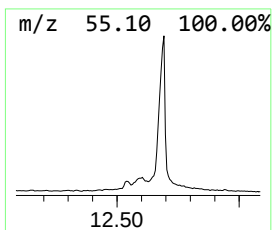
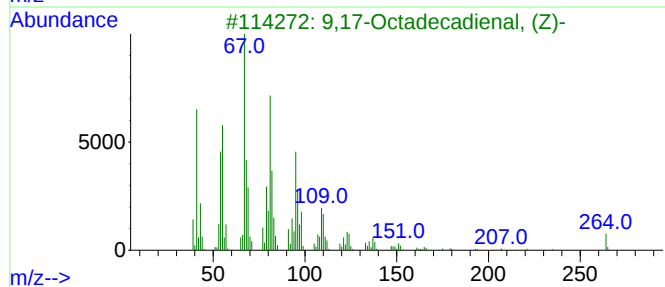
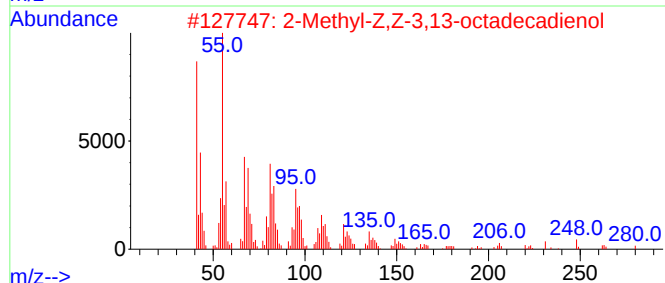
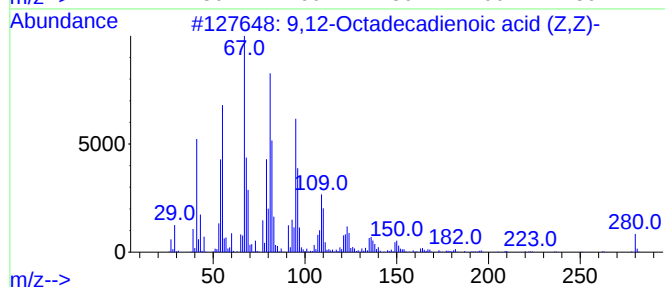
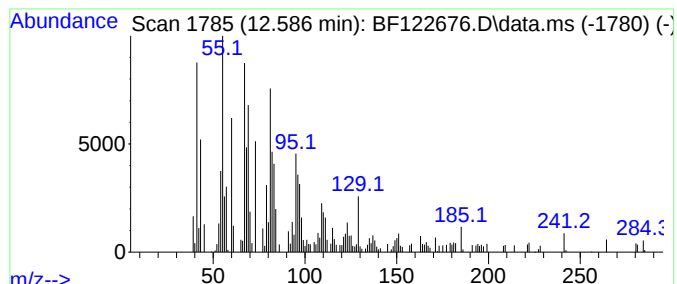
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9,12-Octadecadienoic acid (... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.586	4.32 ng	272594	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	98
2			2-Methyl-Z,Z-3,13-octadecadienol	280	C19H36O	1000130-90-5	86
3			9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	84
4			9-Eicosyne	278	C20H38	071899-38-2	68
5			1,13-Tetradecadiene	194	C14H26	021964-49-8	68



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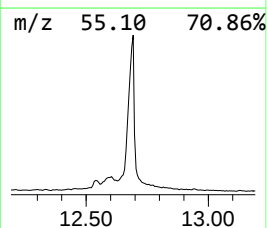
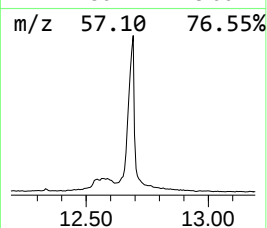
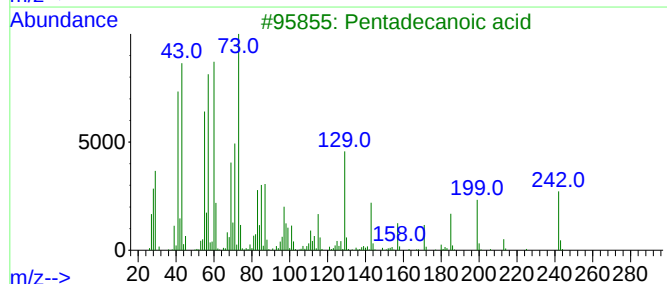
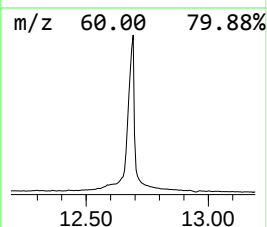
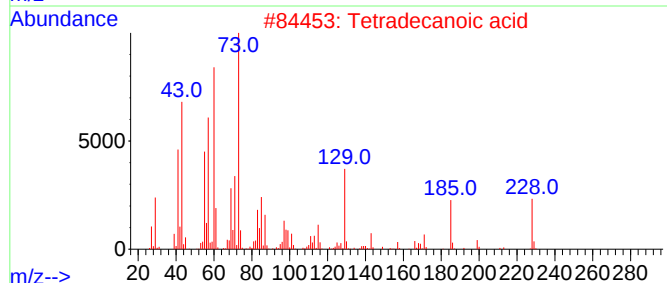
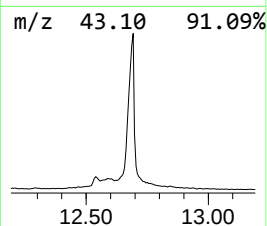
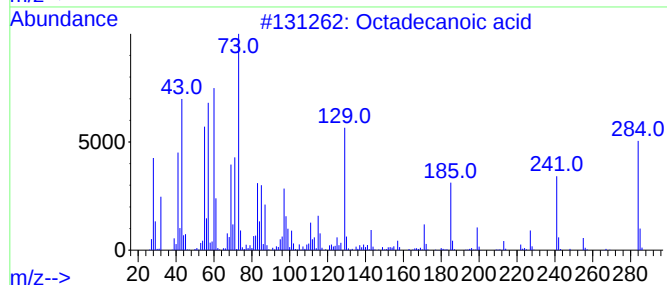
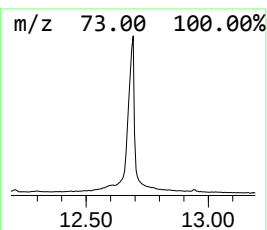
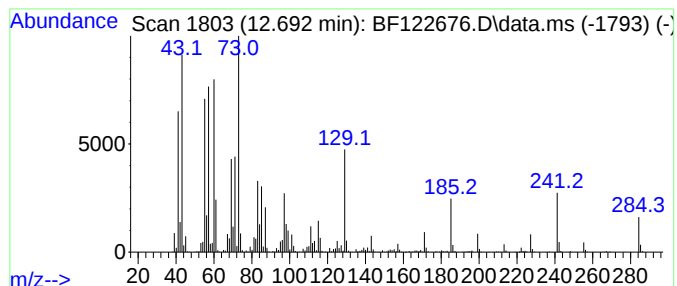
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Peak Number 5 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.692	134.78 ng	8224810	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



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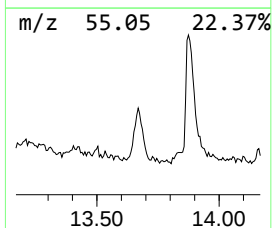
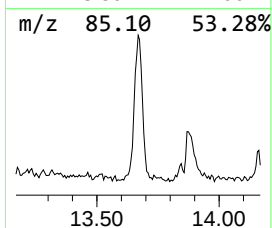
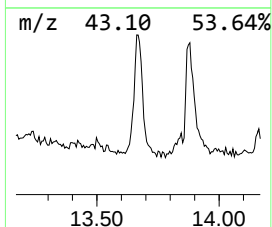
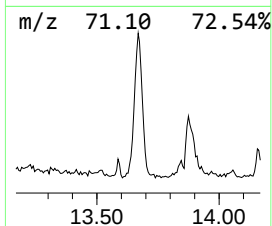
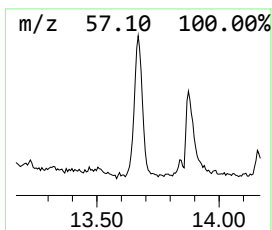
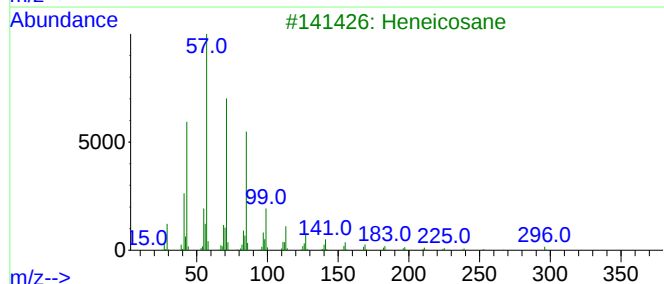
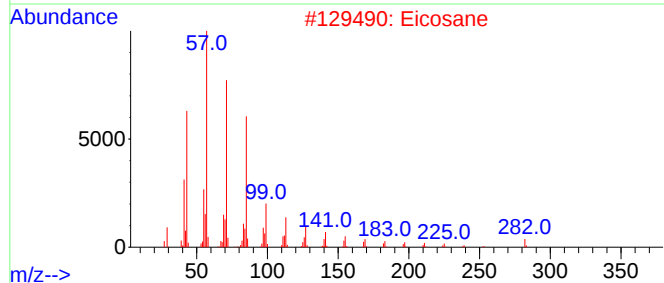
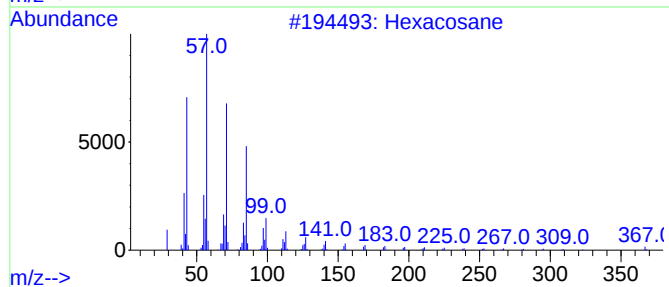
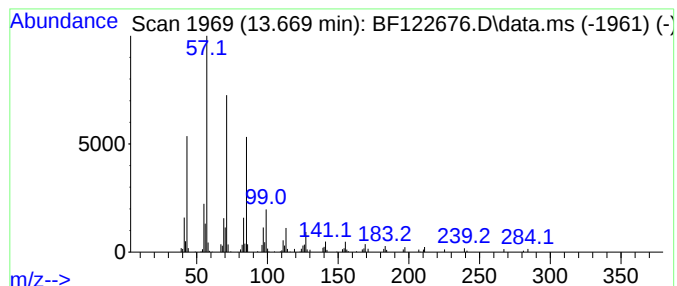
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.669	6.26 ng	382181	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Eicosane	282	C20H42	000112-95-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			2-methyloctacosane	408	C29H60	1000376-72-8	91
5			Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121220\
Data File : BF122676.D
Acq On : 12 Dec 2020 14:04
Operator : JU/CG
Sample : L5042-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KENS-B6-121020-0-6

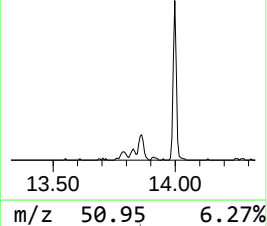
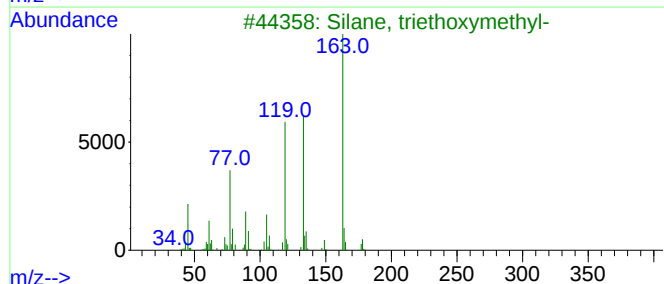
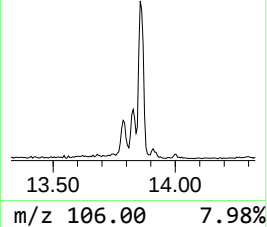
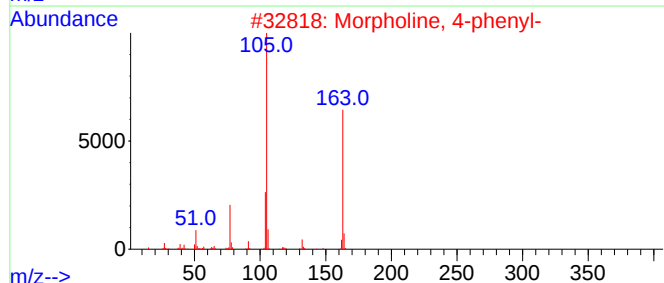
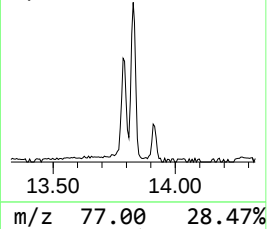
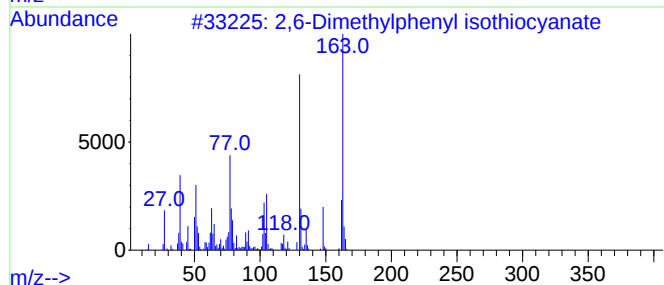
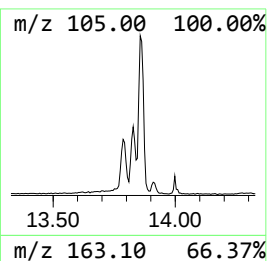
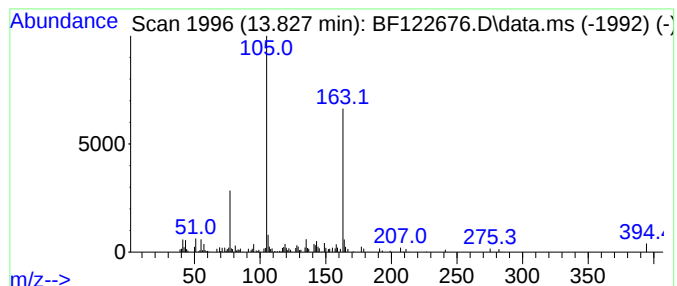
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,6-Dimethylphenyl isothiocy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	2.39 ng	146070	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Dimethylphenyl isothiocyanate	163	C9H9NS	019241-16-8	50
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	50
3			Silane, triethoxymethyl-	178	C7H18O3Si	002031-67-6	43
4			Benzoic acid, 3,3-dimethylbut-2-...	206	C13H18O2	1000368-20-7	27
5			1-Benzoyl-2-trichloroacetylhydra...	280	C9H7Cl3N2O2	090273-66-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121220\
Data File : BF122676.D
Acq On : 12 Dec 2020 14:04
Operator : JU/CG
Sample : L5042-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KENS-B6-121020-0-6

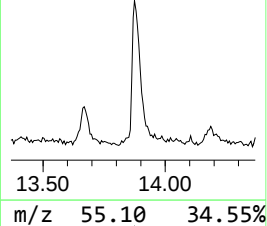
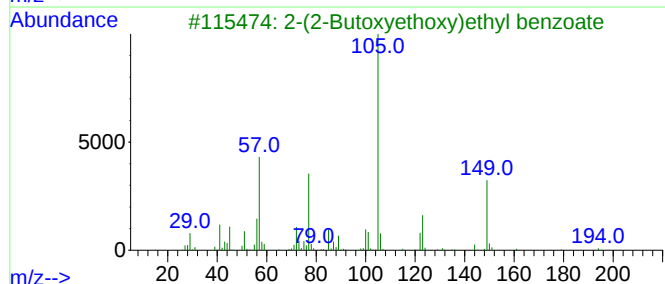
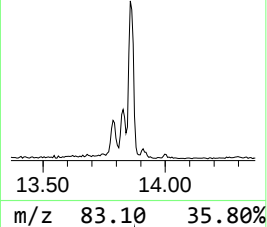
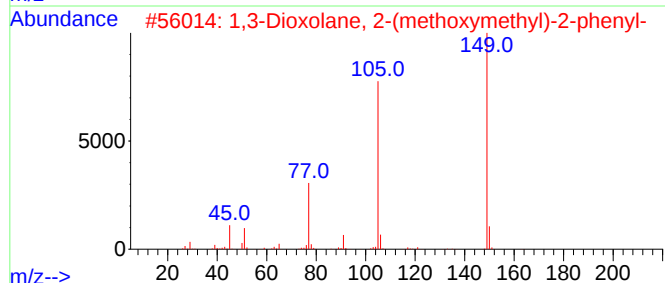
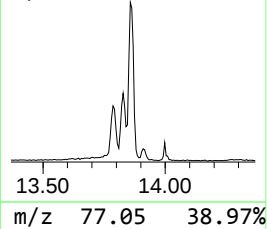
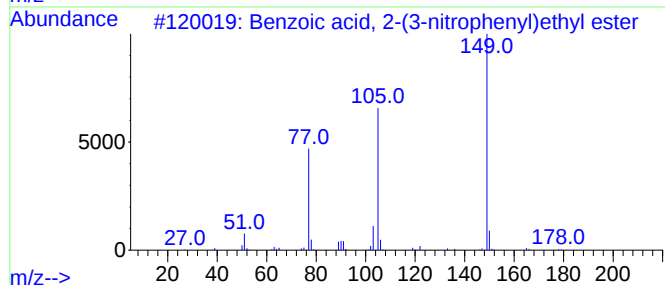
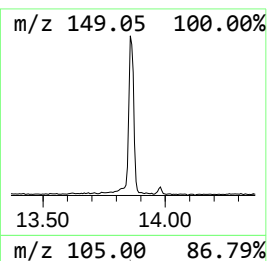
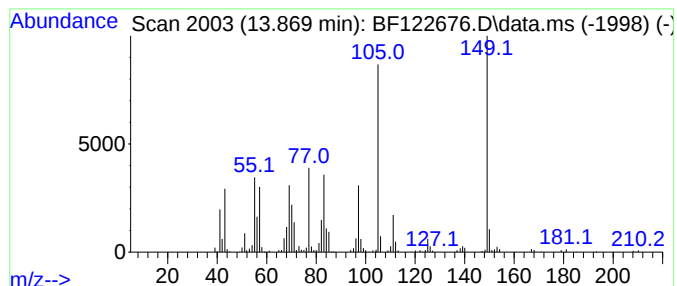
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.868 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	13.46 ng	821097	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	47
2			1,3-Dioxolane, 2-(methoxymethyl)... 194	194	C11H14O3	1000156-71-2	47
3			2-(2-Butoxyethoxy)ethyl benzoate	266	C15H22O4	1000366-98-4	43
4			Benzoic acid, 2-(2-chlorophenoxy...	276	C15H13ClO3	1000368-25-9	40
5			Phthalic acid, propyl octadecyl ...	460	C29H48O4	1000308-96-7	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121220\
Data File : BF122676.D
Acq On : 12 Dec 2020 14:04
Operator : JU/CG
Sample : L5042-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

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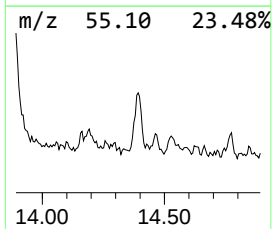
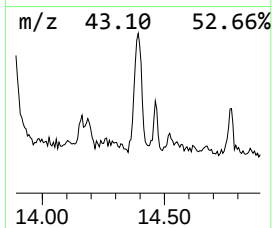
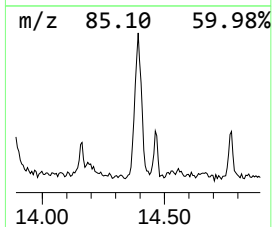
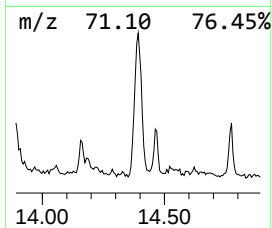
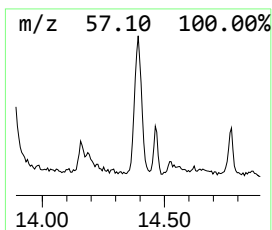
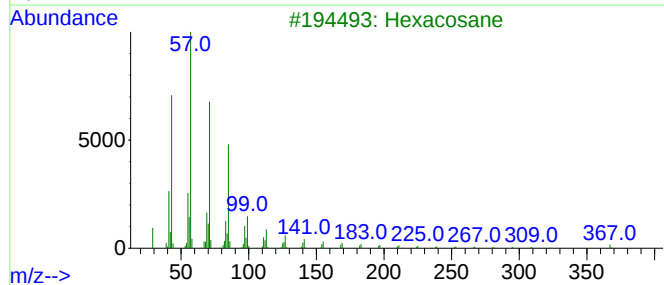
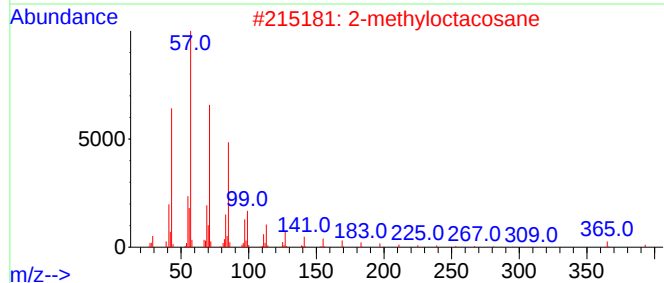
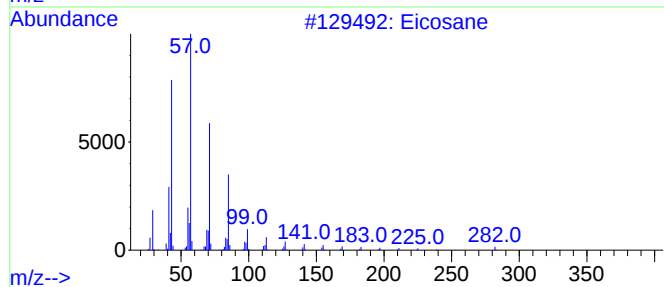
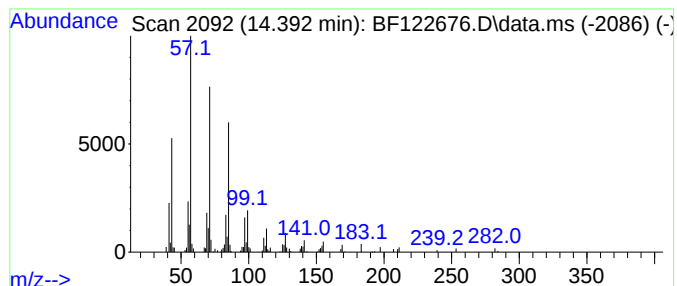
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.392	4.46 ng	272304	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	97
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121220\
Data File : BF122676.D
Acq On : 12 Dec 2020 14:04
Operator : JU/CG
Sample : L5042-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

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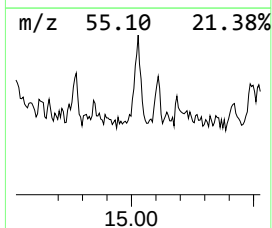
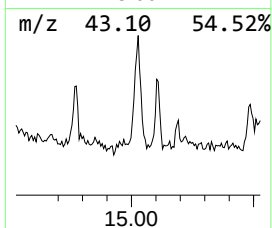
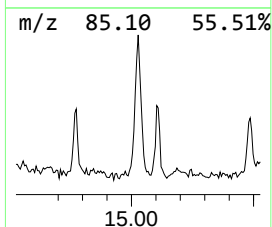
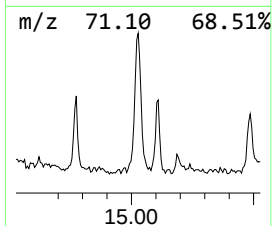
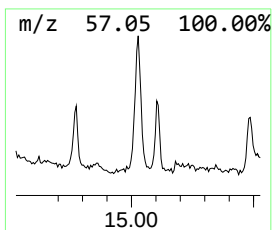
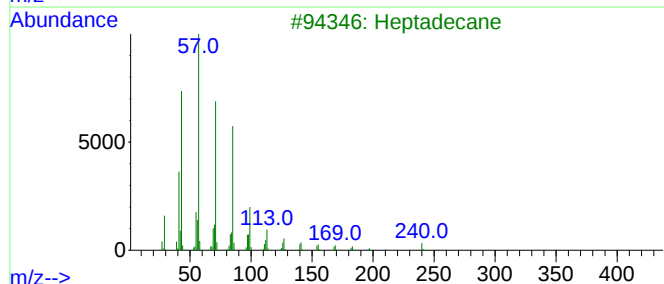
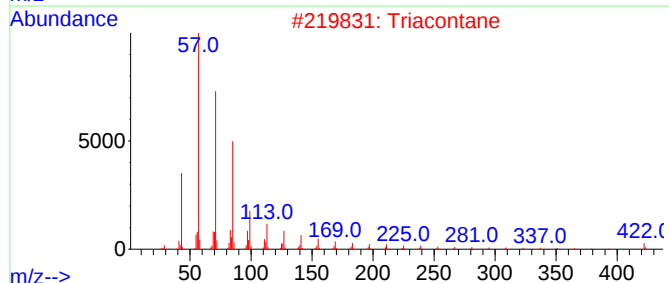
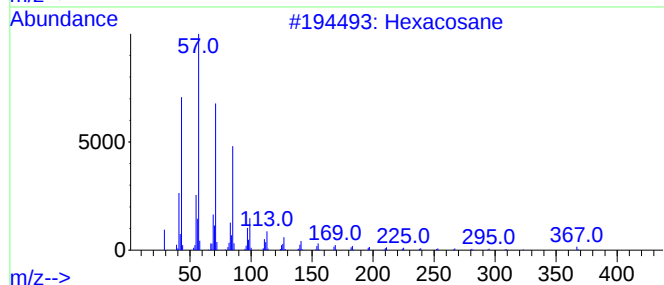
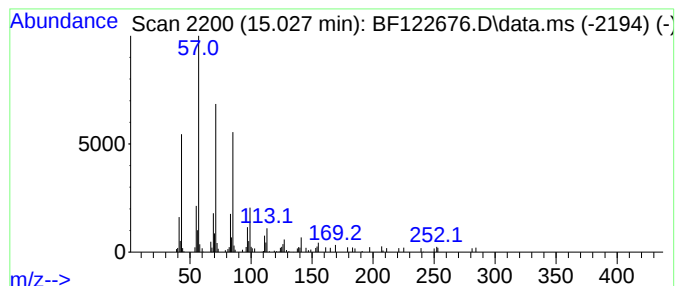
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.027	3.15 ng	178507	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	90
2		Triacotane	422	C30H62	000638-68-6	90
3		Heptadecane	240	C17H36	000629-78-7	87
4		Heneicosane	296	C21H44	000629-94-7	87
5		2-methyloctacosane	408	C29H60	1000376-72-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121220\
Data File : BF122676.D
Acq On : 12 Dec 2020 14:04
Operator : JU/CG
Sample : L5042-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

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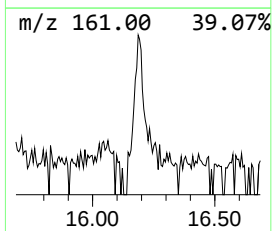
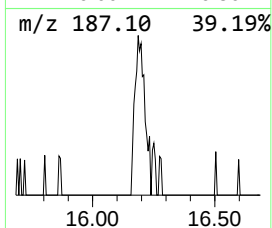
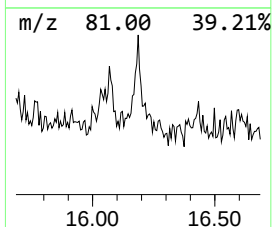
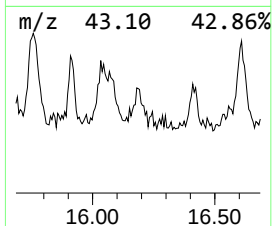
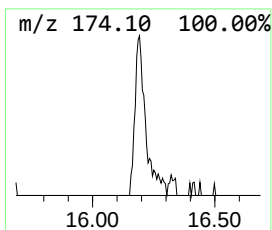
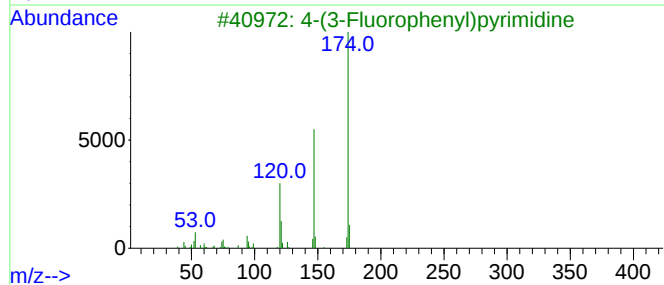
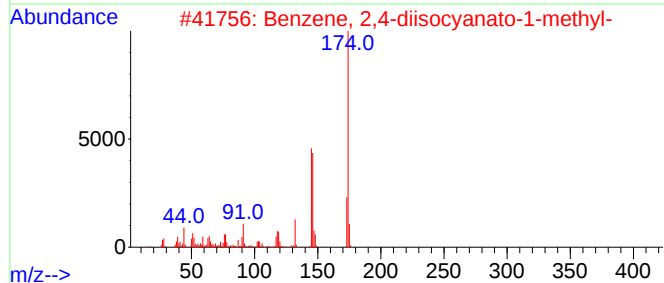
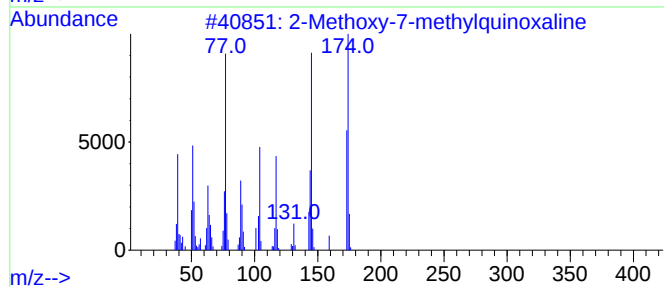
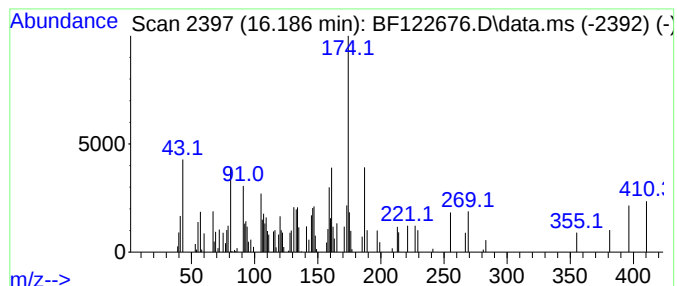
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.186 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.186	2.03 ng	115051	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methoxy-7-methylquinoxaline	174	C10H10N2O	1000103-05-6	25
2			Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	25
3			4-(3-Fluorophenyl)pyrimidine	174	C10H7FN2	068049-18-3	22
4			s-Indacen-4-ol, 1,2,3,5,6,7-hexa...	216	C14H16O2	063089-53-2	22
5			5-Methyl-5,8-dihydro-1,4-naphtho...	174	C11H10O2	086759-40-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121220\
Data File : BF122676.D
Acq On : 12 Dec 2020 14:04
Operator : JU/CG
Sample : L5042-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KENS-B6-121020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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n-Hexadecanoic ...	11.898	76.5	ng	4831270	4	11.357	1263420	20.0
Methyl stearate	12.539	6.3	ng	394557	4	11.357	1263420	20.0
9,12-Octadecadi...	12.586	4.3	ng	272594	4	11.357	1263420	20.0
Octadecanoic acid	12.692	134.8	ng	8224810	5	13.998	1220500	20.0
Eicosane	13.669	6.3	ng	382181	5	13.998	1220500	20.0
2,6-Dimethylphe...	13.827	2.4	ng	146070	5	13.998	1220500	20.0
unknown13.868	13.868	13.5	ng	821097	5	13.998	1220500	20.0
2-methyloctacosane	14.392	4.5	ng	272304	5	13.998	1220500	20.0
Hexacosane	15.027	3.1	ng	178507	6	15.463	1134880	20.0
unknown16.186	16.186	2.0	ng	115051	6	15.463	1134880	20.0