

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
 Data File : BF128604.D
 Acq On : 31 May 2022 19:59
 Operator : CG\JU
 Sample : N2952-12
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P037-SS001-1218-02

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128604.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.504	542	547	560	rBV	2003763	2113310	84.52%	11.824%
2	6.528	717	721	730	rBV	1929935	2092512	83.69%	11.708%
3	6.840	771	774	778	rBV	721510	629144	25.16%	3.520%
4	7.410	865	871	873	rBV	1513887	1475447	59.01%	8.255%
5	8.128	988	993	996	rBV	871170	753352	30.13%	4.215%
6	9.204	1170	1176	1179	rBV	3140849	2500462	100.00%	13.991%
7	9.881	1287	1291	1295	rBV	927507	768990	30.75%	4.303%
8	10.681	1423	1427	1436	rBV	1174312	1182739	47.30%	6.618%
9	10.786	1442	1445	1455	rVB6	31418	67949	2.72%	0.380%
10	11.010	1477	1483	1491	rVB6	28168	70216	2.81%	0.393%
11	11.369	1541	1544	1548	rBV	809891	654112	26.16%	3.660%
12	11.933	1633	1640	1643	rBV7	46651	113679	4.55%	0.636%
13	12.092	1665	1667	1670	rBV2	34562	32638	1.31%	0.183%
14	12.575	1745	1749	1755	rVB2	283087	415852	16.63%	2.327%
15	12.957	1810	1814	1818	rBV	2066672	2016622	80.65%	11.283%
16	13.039	1824	1828	1835	rBV7	36904	83437	3.34%	0.467%
17	13.351	1877	1881	1890	rVB2	225122	352900	14.11%	1.975%
18	13.592	1918	1922	1929	rVB	296644	462906	18.51%	2.590%
19	14.010	1990	1993	1997	rBV	588703	553276	22.13%	3.096%
20	14.057	1997	2001	2006	rVV2	187780	272688	10.91%	1.526%
21	14.116	2008	2011	2019	rVB	230195	253954	10.16%	1.421%
22	14.292	2037	2041	2046	rVB	174735	221247	8.85%	1.238%
23	14.721	2110	2114	2119	rBV3	125628	183269	7.33%	1.025%
24	14.974	2153	2157	2166	rVB	101408	188144	7.52%	1.053%
25	15.486	2239	2244	2248	rBV	330637	413710	16.55%	2.315%

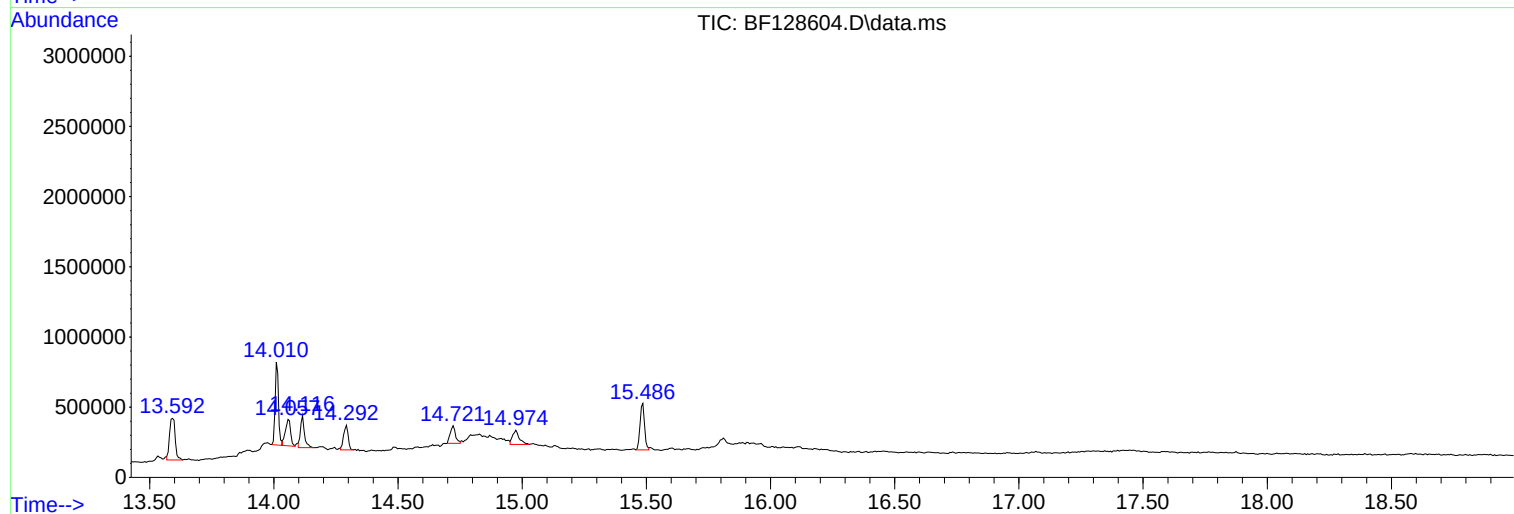
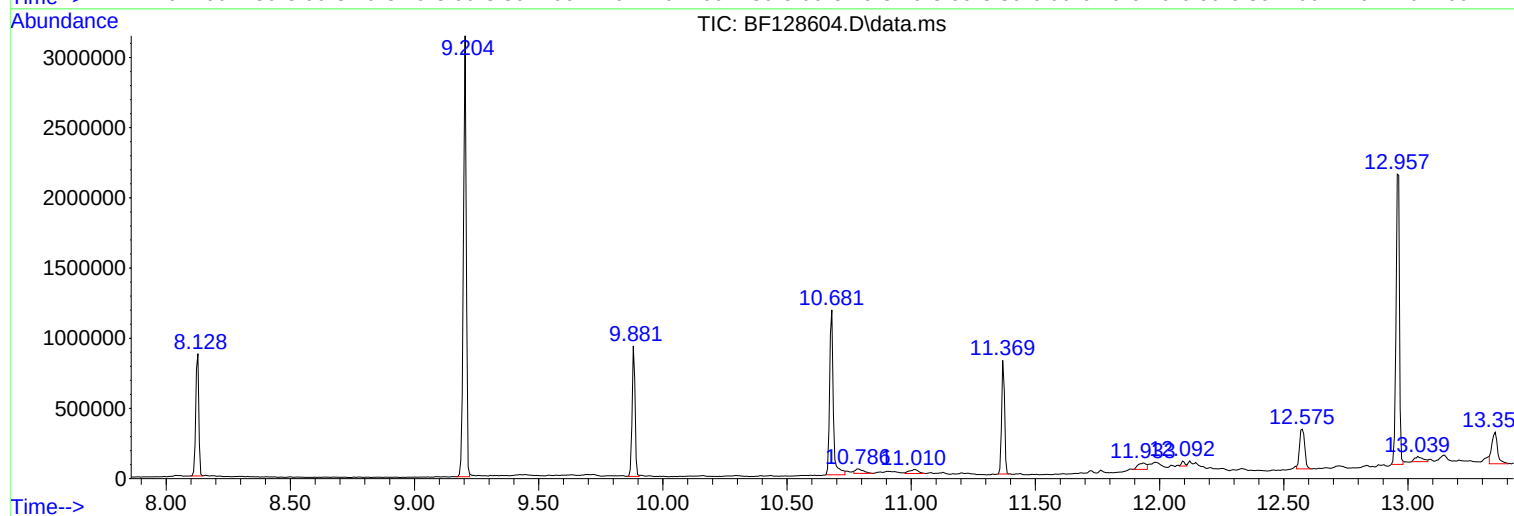
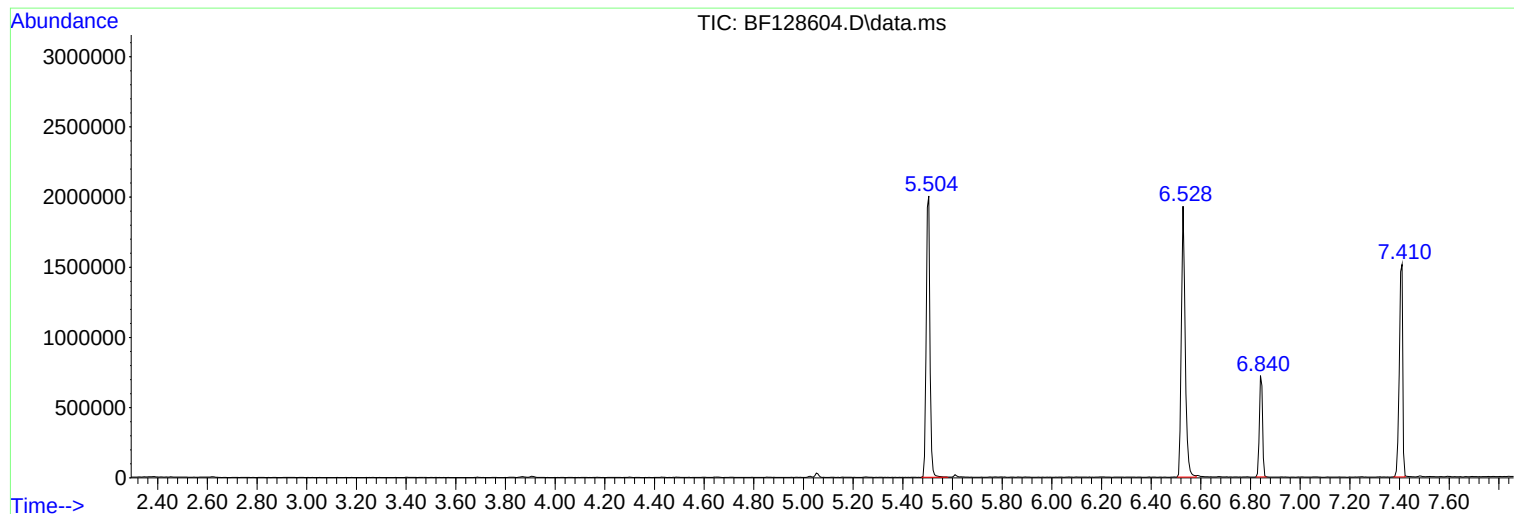
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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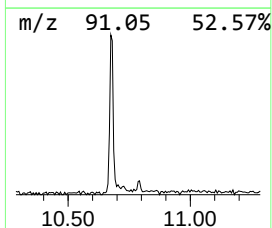
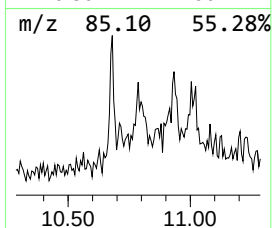
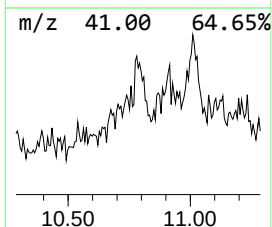
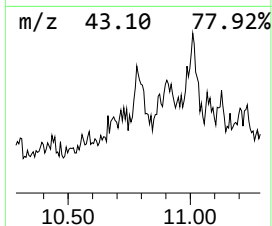
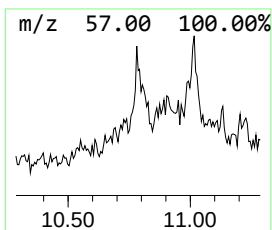
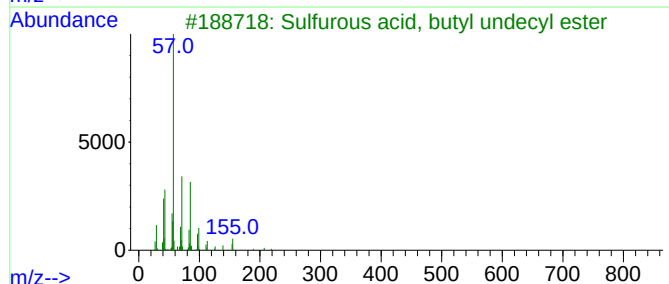
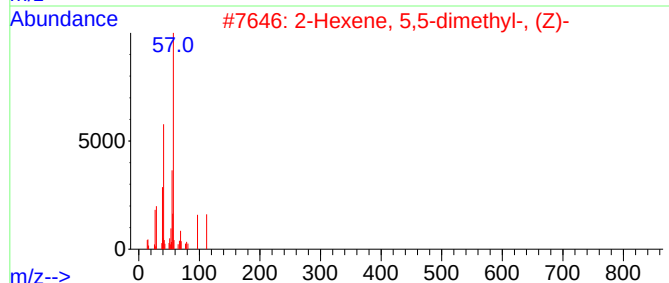
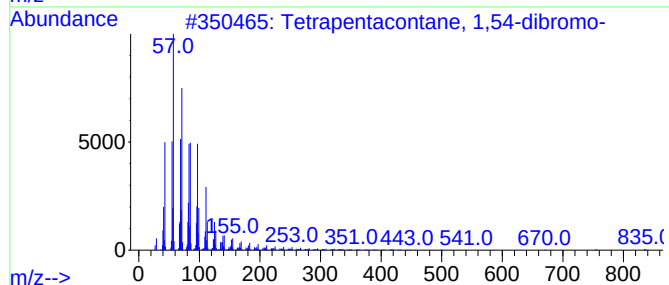
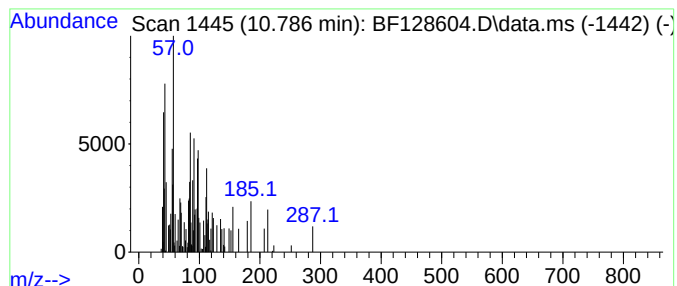
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown10.786 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.786	2.08 ng	67949	Phenanthrene-d10	11.369	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	27
2	2-Hexene, 5,5-dimethyl-, (Z)-	112	C8H16	039761-61-0	14
3	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	14
4	3-Hexen-2-one, 5-methyl-	112	C7H12O	005166-53-0	14
5	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	14



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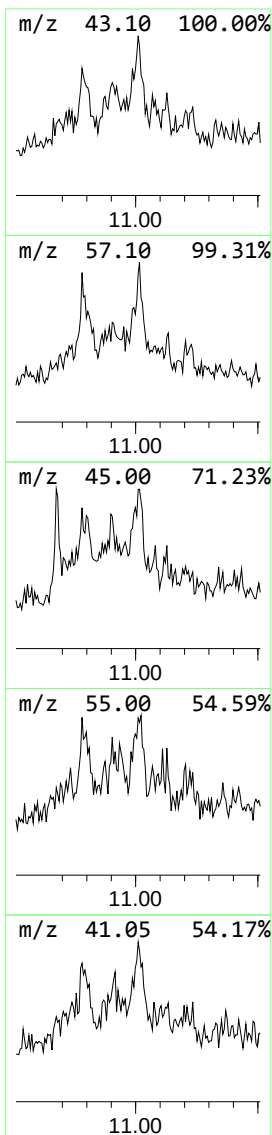
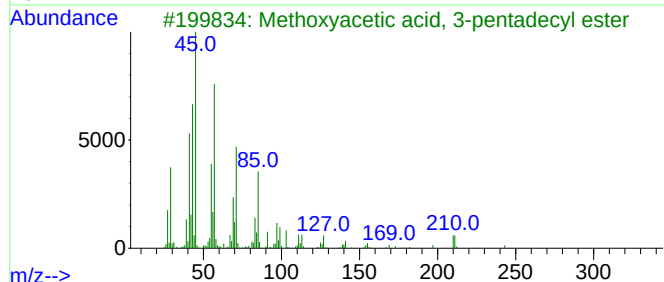
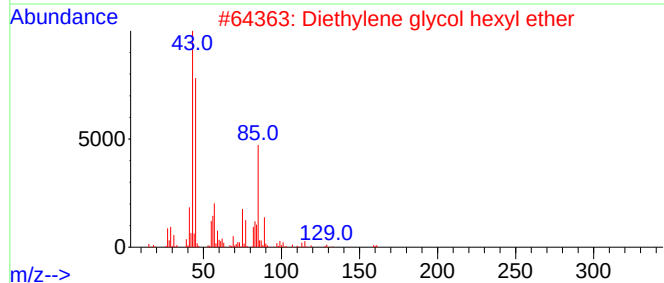
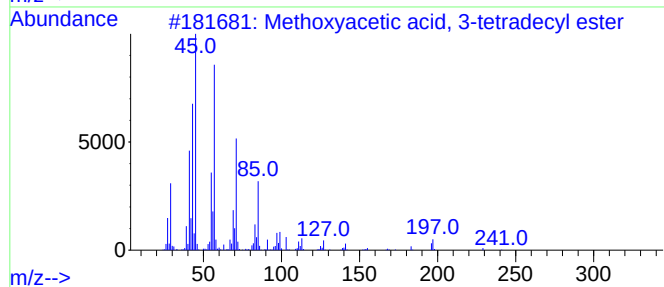
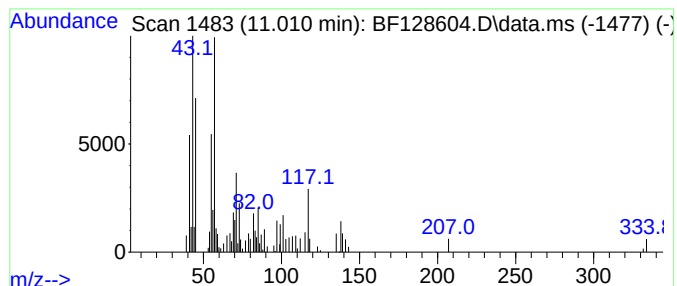
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown11.010 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.010	2.15 ng	70216	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methoxyacetic acid, 3-tetradecyl...	286	C17H34O3	1000282-04-9	35
2			Diethylene glycol hexyl ether	190	C10H22O3	000112-59-4	35
3			Methoxyacetic acid, 3-pentadecyl...	300	C18H36O3	1010282-05-2	35
4			2H-Pyran-2-methanol, 3,6-dihydro...	188	C9H16O4	056196-34-0	35
5			Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	35



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Misc :
ALS Vial : 13 Sample Multiplier: 1

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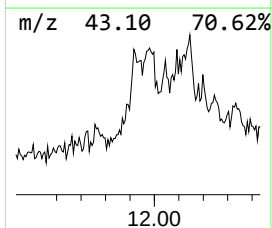
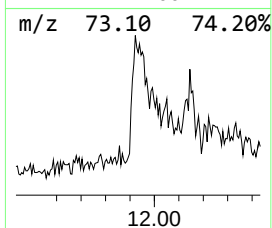
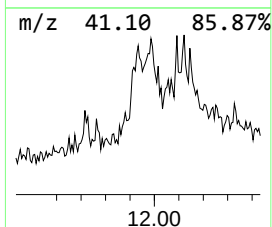
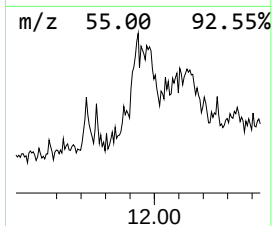
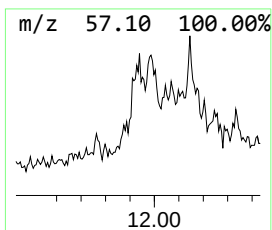
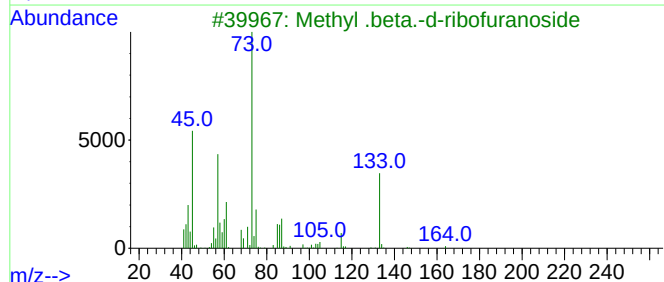
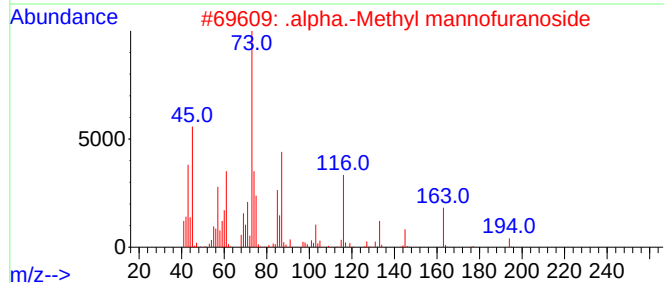
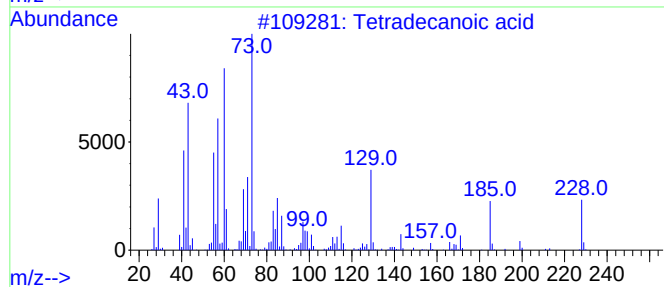
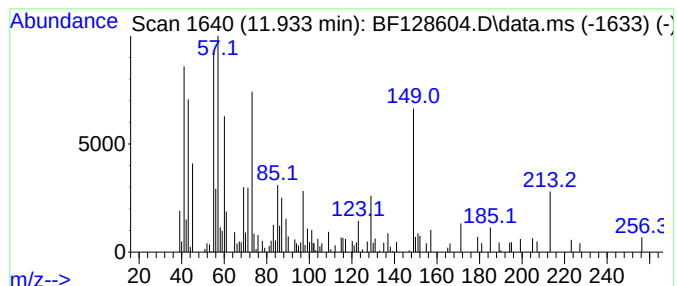
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown11.933 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	3.48 ng	113679	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	27
2			.alpha.-Methyl mannofuranoside	194	C7H14O6	004097-91-0	27
3			Methyl .beta.-d-ribofuranoside	164	C6H12O5	1000129-84-0	22
4			5-Chloro-2-methyl-3(2H)-isothiaz...	149	C4H4ClNOS	026172-55-4	22
5			Phthalic acid, isobutyl 2-(2-met...	364	C21H32O5	1000314-93-8	22



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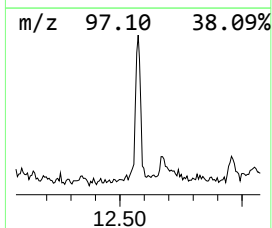
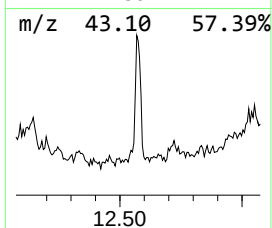
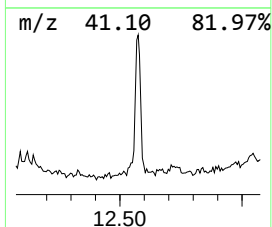
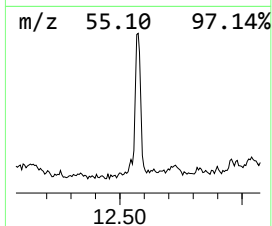
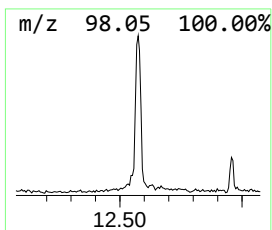
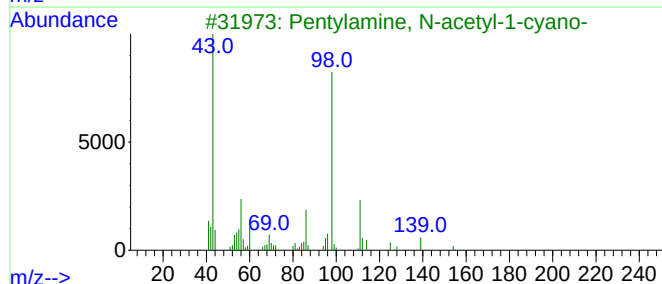
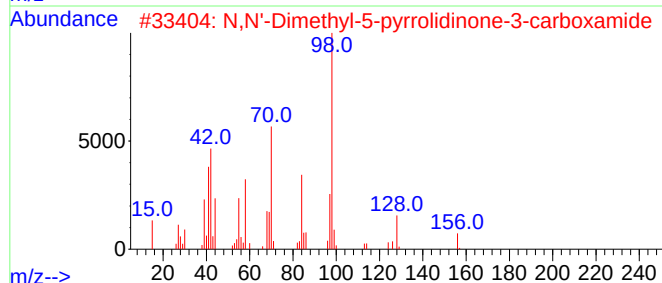
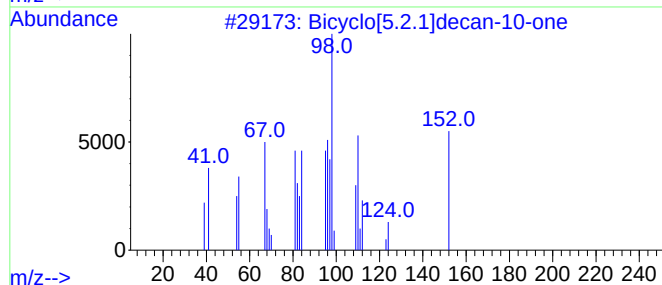
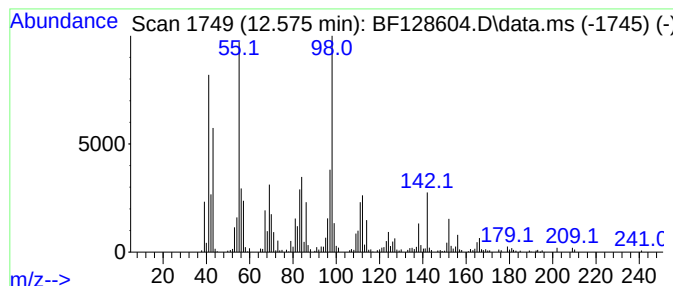
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Bicyclo[5.2.1]decan-10-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.575	12.72 ng	415852	Phenanthrene-d10		11.369	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Bicyclo[5.2.1]decan-10-one		152	C10H16O	004696-15-5	50
2	N,N'-Dimethyl-5-pyrrolidinone-3-...		156	C7H12N2O2	089851-99-0	47
3	Pentylamine, N-acetyl-1-cyano-		154	C8H14N2O	027395-08-0	38
4	Propionamide, 3-(1-piperidyl)-		156	C8H16N2O	004269-30-1	35
5	Pyrrolid-2-one-5-methanol, N-met...		171	C8H13NO3	1000125-92-2	27



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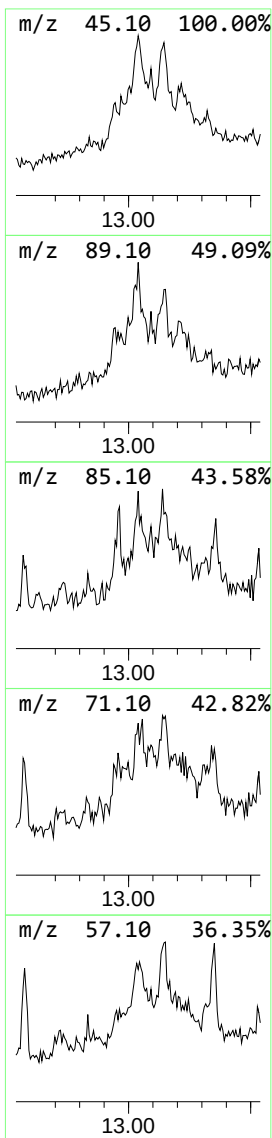
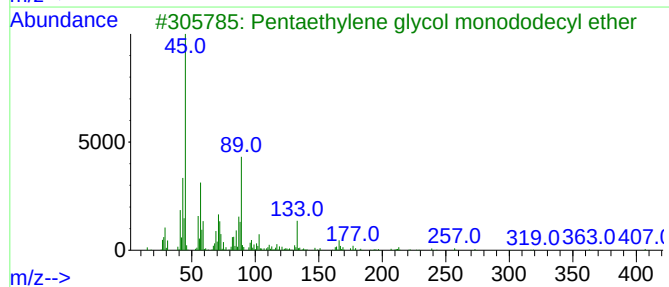
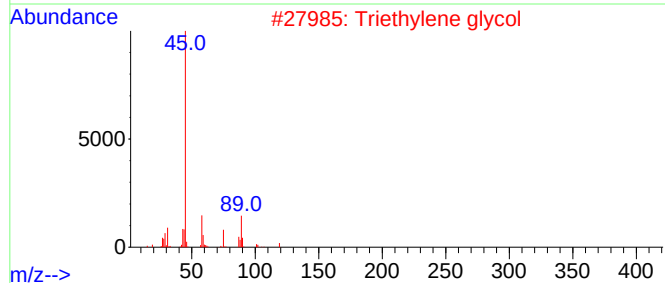
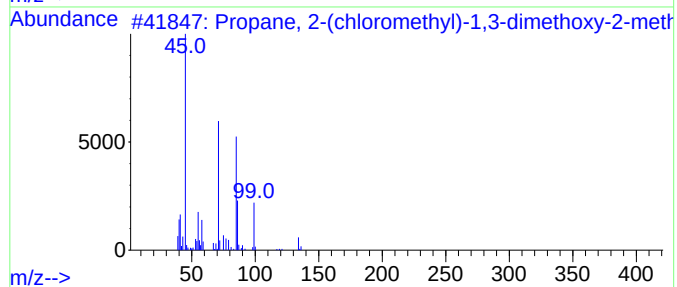
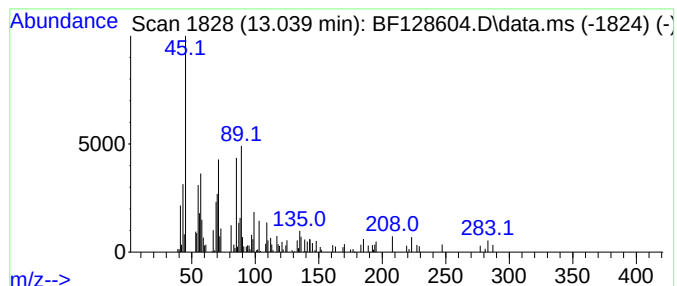
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Peak Number 5 Propane, 2-(chloromethyl)-1... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.039	3.02 ng	83437	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-(chloromethyl)-1,3-di...	166	C7H15ClO2	020637-37-0	50
2	Triethylene glycol	150	C6H14O4	000112-27-6	38
3	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	37
4	1-Pentanol, 5-methoxy-	118	C6H14O2	004799-62-6	32
5	1,4,7,10,13,16-Hexaoxanonadecane...	320	C16H32O6	1000163-65-3	32



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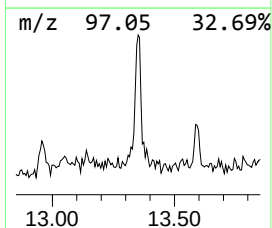
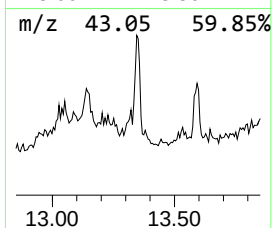
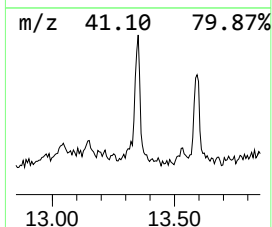
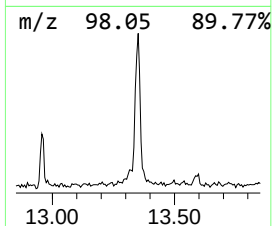
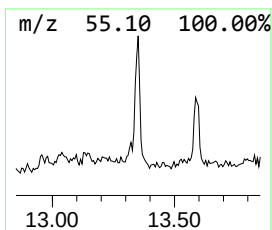
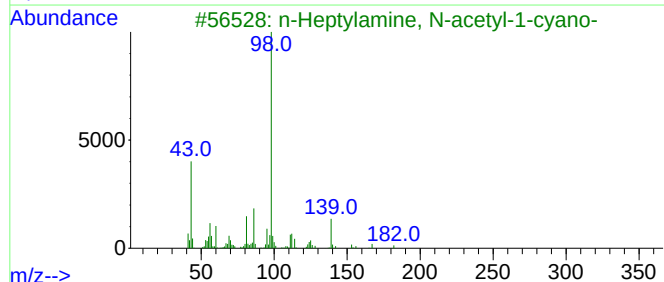
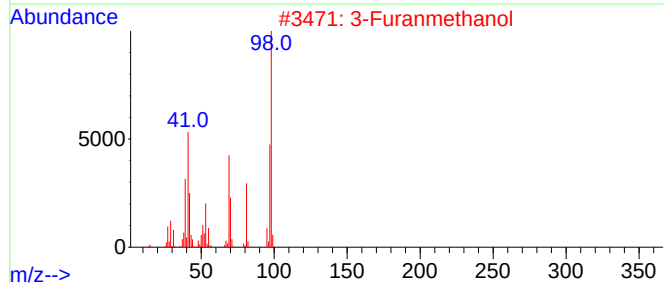
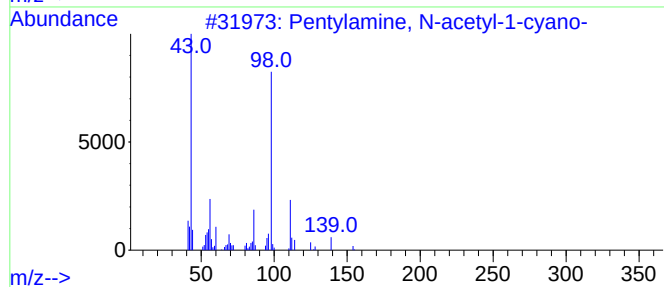
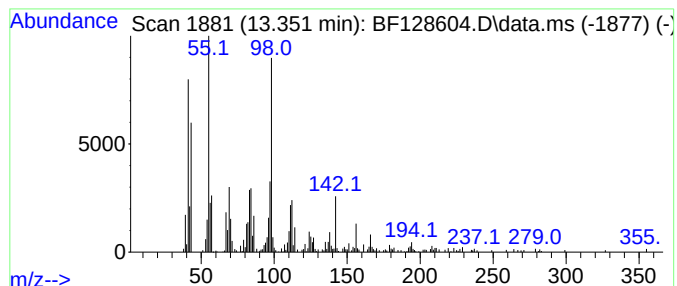
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Peak Number 6 unknown13.351 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.351	12.76 ng	352900	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentylamine, N-acetyl-1-cyano-	154	C8H14N2O	027395-08-0	43
2			3-Furanmethanol	98	C5H6O2	004412-91-3	38
3			n-Heptylamine, N-acetyl-1-cyano-	182	C10H18N2O	1000227-03-9	38
4			Cyclohexanone, 2-propyl-	140	C9H16O	000094-65-5	35
5			2-Pentenal, 2-methyl-	98	C6H10O	000623-36-9	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128604.D
Acq On : 31 May 2022 19:59
Operator : CG\JU
Sample : N2952-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P037-SS001-1218-02

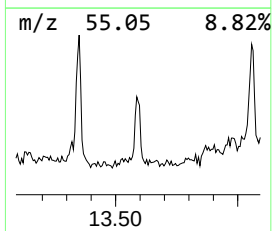
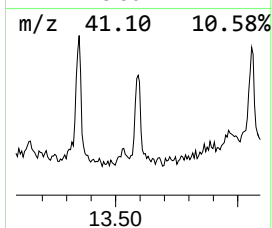
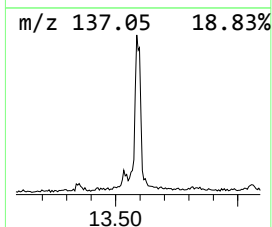
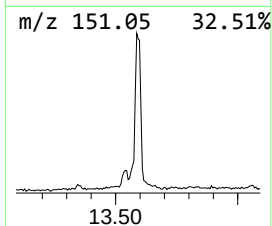
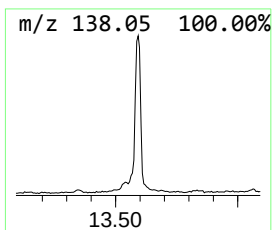
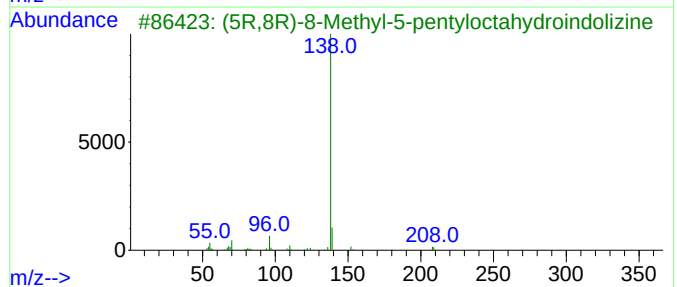
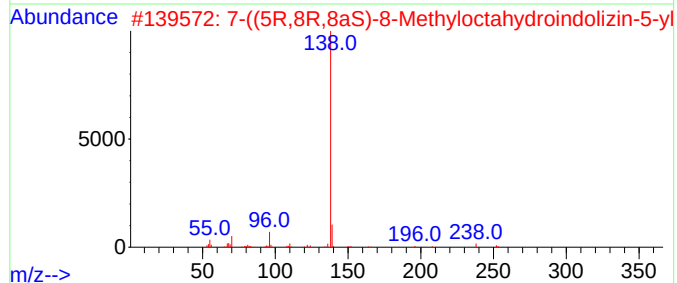
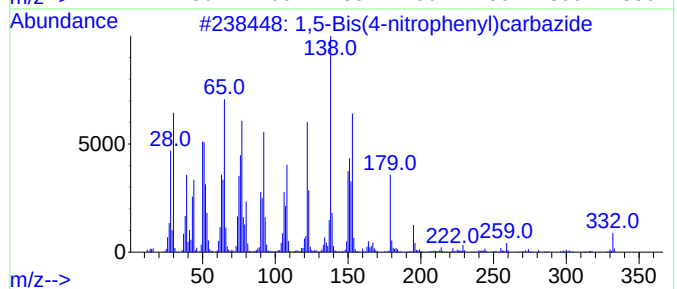
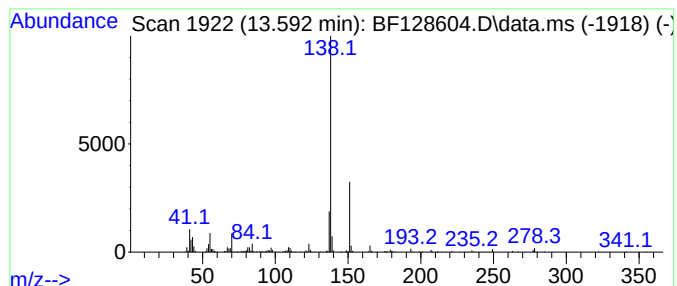
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.592 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.592	16.73 ng	462906	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5-Bis(4-nitrophenyl)carbazide	332	C13H12N6O5	000622-69-5	47
2			7-((5R,8R,8aS)-8-Methyloctahydro...	253	C16H31NO	1000367-28-5	47
3			(5R,8R)-8-Methyl-5-pentyloctahyd...	209	C14H27N	117959-79-2	47
4			2,5-Cyclohexadiene-1,4-dione, 2-...	138	C7H6O3	000615-91-8	47
5			Succinic acid, 3-methylbut-2-en-...	306	C17H22O5	1000390-95-6	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128604.D
Acq On : 31 May 2022 19:59
Operator : CG\JU
Sample : N2952-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P037-SS001-1218-02

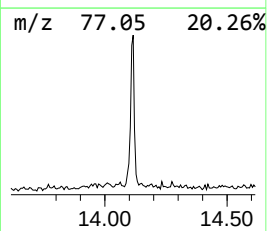
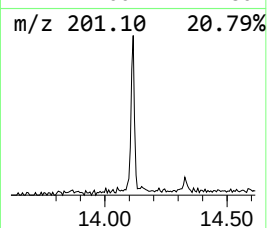
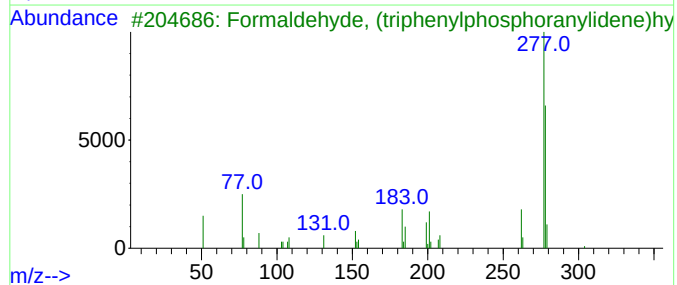
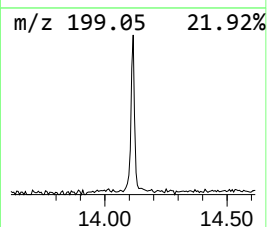
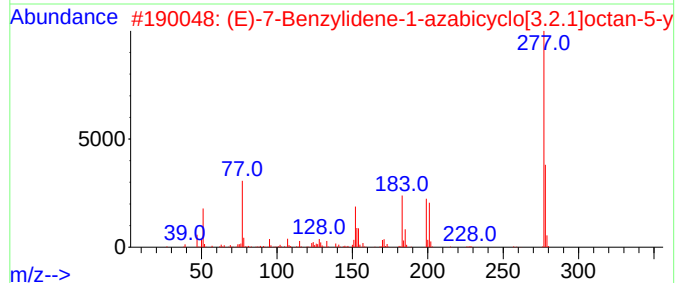
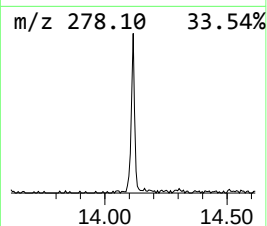
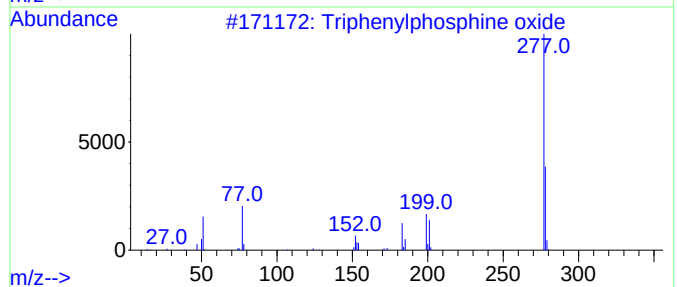
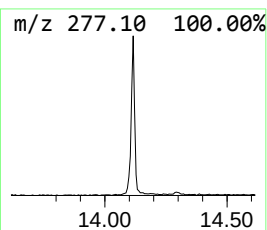
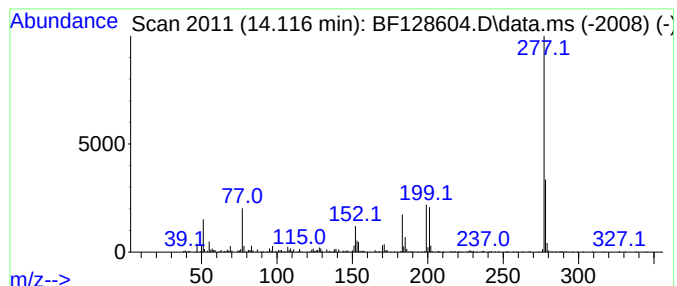
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.116	9.18 ng	253954	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	72
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	45
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
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Sample : N2952-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P037-SS001-1218-02

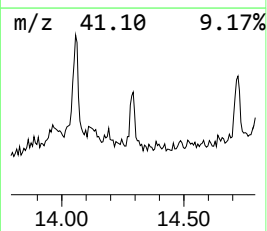
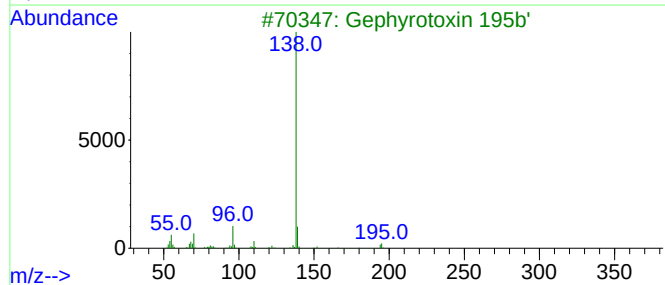
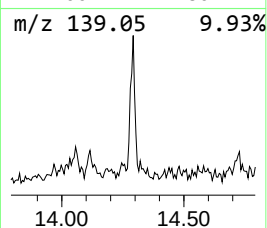
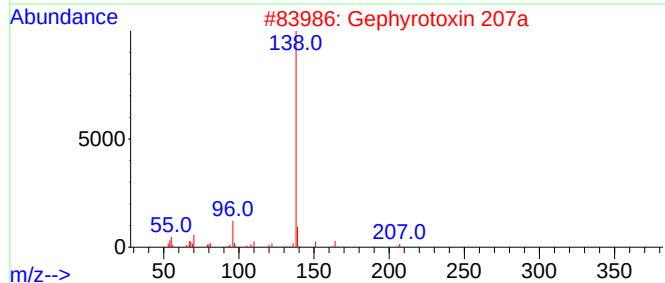
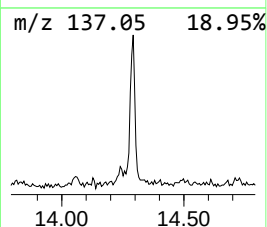
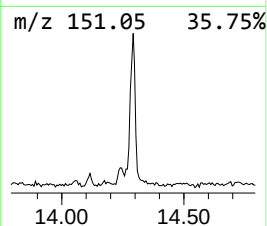
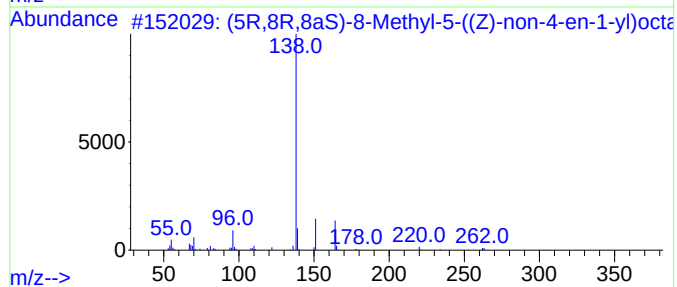
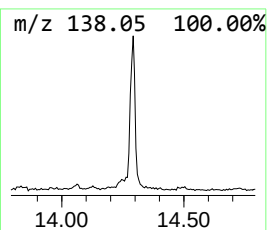
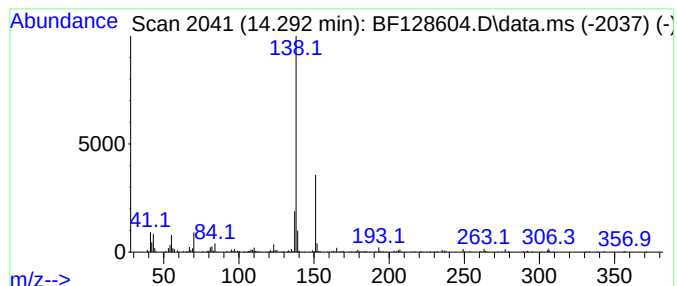
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 (5R,8R,8aS)-8-Methyl-5-((Z)... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.292	8.00 ng	221247	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(5R,8R,8aS)-8-Methyl-5-((Z)-non-...	263	C18H33N	1000367-14-0	58
2			Gephyrotoxin 207a	207	C14H25N	141724-48-3	52
3			Gephyrotoxin 195b'	195	C13H25N	1000116-01-4	50
4			(5R,8R,8aS)-8-Methyl-5-(pent-4-y...	205	C14H23N	109175-46-4	50
5			Succinic acid, dodec-2-en-1-yl 2...	404	C24H36O5	1000390-96-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128604.D
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Sample : N2952-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

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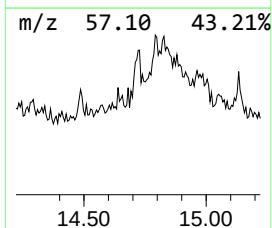
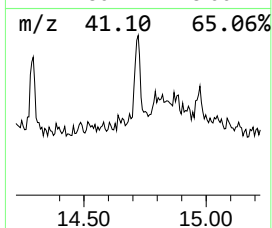
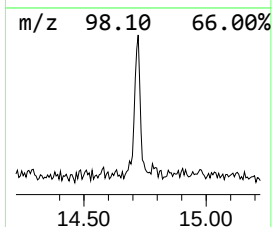
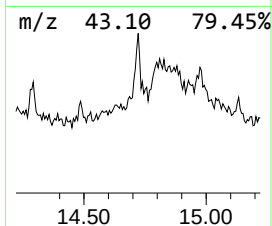
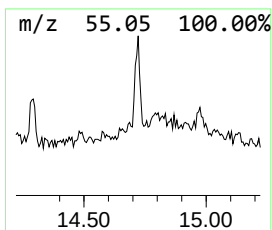
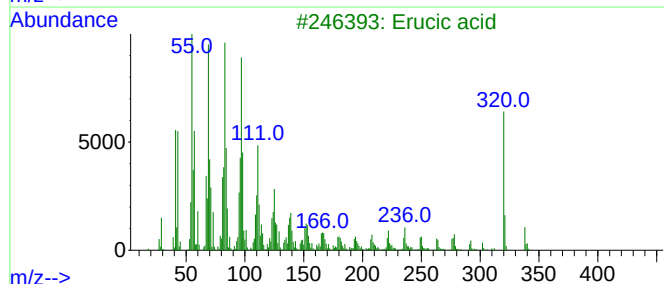
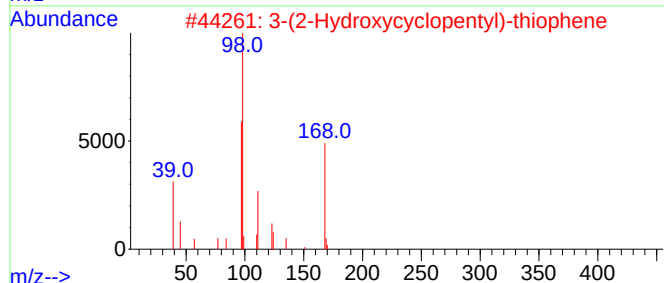
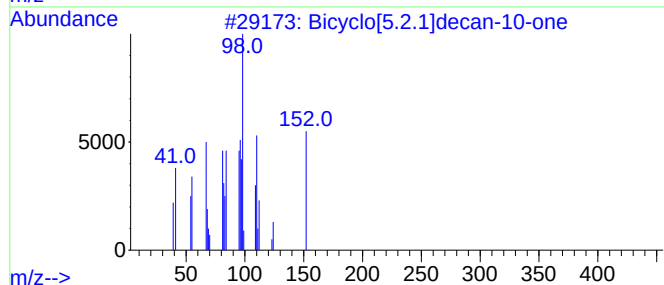
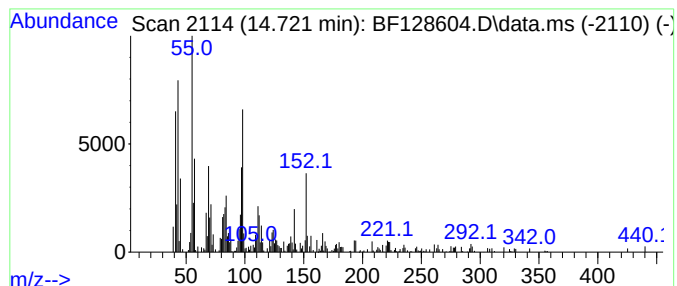
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.722 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.722	6.62 ng	183269	Chrysene-d12	14.010

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[5.2.1]decan-10-one	152	C10H16O	004696-15-5	46
2		3-(2-Hydroxycyclopentyl)-thiophene	168	C9H12OS	1000145-10-2	43
3		Erucic acid	338	C22H42O2	000112-86-7	43
4		But-2-enedioic acid, diamide	114	C4H6N2O2	1010192-49-3	43
5		2-Oxecanone, 10-methyl-, (+/-)-	170	C10H18O2	065371-24-6	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128604.D
Acq On : 31 May 2022 19:59
Operator : CG\JU
Sample : N2952-12
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Instrument :
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ClientSampleId :
P037-SS001-1218-02

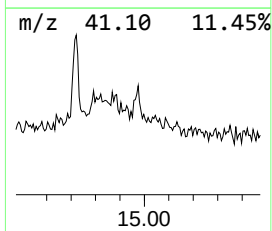
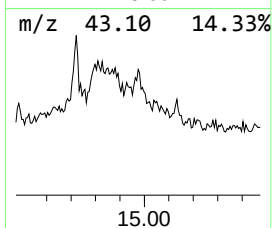
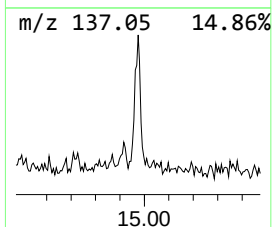
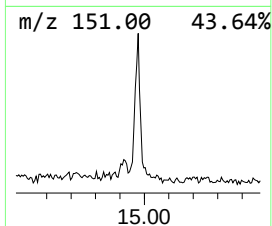
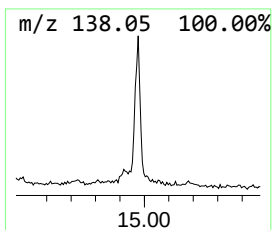
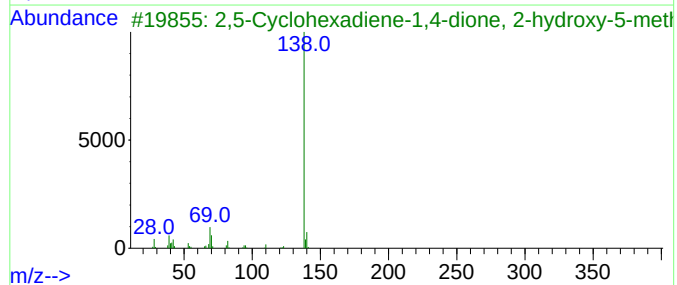
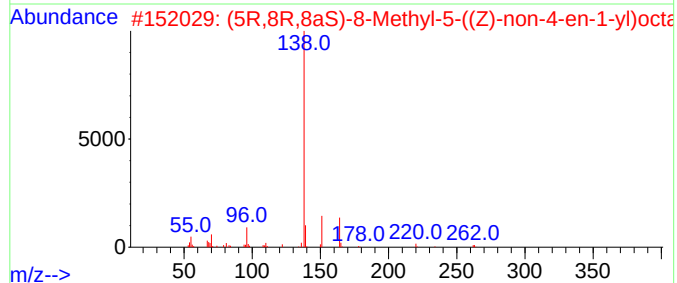
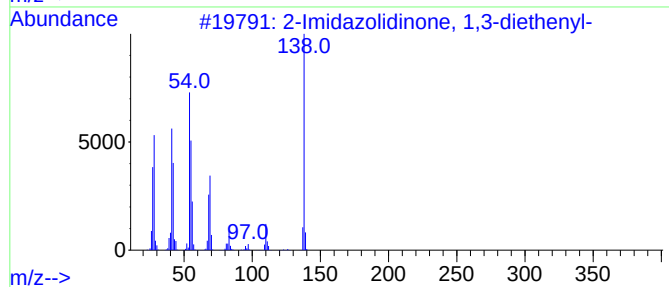
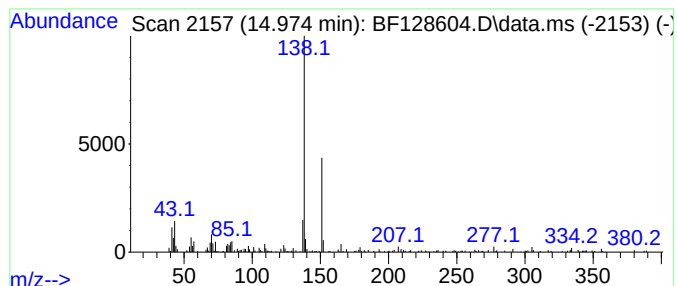
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown14.974 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	9.10 ng	188144	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Imidazolidinone, 1,3-diethenyl-	138	C7H10N2O	013811-50-2	47		
2	(5R,8R,8aS)-8-Methyl-5-((Z)-non-...	263	C18H33N	1000367-14-0	47		
3	2,5-Cyclohexadiene-1,4-dione, 2-...	138	C7H6O3	000615-91-8	46		
4	Succinic acid, 2,2-dichloroethyl...	334	C14H16Cl2O5	1000390-95-7	43		
5	Glutaric acid, 2-(3-chlorophenyl...	494	C29H47ClO4	1010377-29-6	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
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Sample : N2952-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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--			
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unknown11.010	11.010	2.1	ng	70216	4	11.369	654112	20.0
unknown11.933	11.933	3.5	ng	113679	4	11.369	654112	20.0
Bicyclo[5.2.1]d...	12.575	12.7	ng	415852	4	11.369	654112	20.0
Propane, 2-(chl...	13.039	3.0	ng	83437	5	14.010	553276	20.0
unknown13.351	13.351	12.8	ng	352900	5	14.010	553276	20.0
unknown13.592	13.592	16.7	ng	462906	5	14.010	553276	20.0
Triphenylphosph...	14.116	9.2	ng	253954	5	14.010	553276	20.0
(5R,8R,8aS)-8-M...	14.292	8.0	ng	221247	5	14.010	553276	20.0
unknown14.722	14.722	6.6	ng	183269	5	14.010	553276	20.0
unknown14.974	14.974	9.1	ng	188144	6	15.486	413710	20.0