

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060222\
 Data File : BF128651.D
 Acq On : 02 Jun 2022 21:40
 Operator : CG\JU
 Sample : N2988-24
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P015-SS006-0006-01

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: BF128651.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	466	470	475	rVB	33479	41678	1.32%	0.200%
2	5.475	538	542	550	rBV	2394101	2371221	75.34%	11.383%
3	6.445	703	707	710	rBV	42811	34243	1.09%	0.164%
4	6.487	710	714	724	rBV	2606867	2452722	77.93%	11.774%
5	6.822	767	771	774	rBV	906642	727919	23.13%	3.494%
6	7.387	861	867	870	rBV	1699531	1670648	53.08%	8.020%
7	7.504	882	887	891	rBV2	55843	54324	1.73%	0.261%
8	8.104	983	989	993	rBV	1063528	929192	29.52%	4.460%
9	9.186	1166	1173	1176	rBV	3415999	3147226	100.00%	15.108%
10	9.863	1282	1288	1291	rBV	1261642	1066313	33.88%	5.119%
11	10.657	1414	1423	1426	rBV	1844232	1673854	53.19%	8.035%
12	11.351	1536	1541	1544	rBV	1347381	1088550	34.59%	5.225%
13	11.880	1628	1631	1635	rBV	35780	34616	1.10%	0.166%
14	12.939	1806	1811	1815	rBV	3054718	3021544	96.01%	14.505%
15	13.898	1967	1974	1975	rBV	71087	112087	3.56%	0.538%
16	13.992	1986	1990	1994	rVB	906327	788421	25.05%	3.785%
17	14.086	2000	2006	2011	rBV	174465	207544	6.59%	0.996%
18	14.468	2068	2071	2075	rBV	40811	35294	1.12%	0.169%
19	15.115	2177	2181	2185	rVB	55988	59059	1.88%	0.284%
20	15.457	2234	2239	2243	rBV	467372	559673	17.78%	2.687%
21	15.933	2314	2320	2327	rBV	58926	88307	2.81%	0.424%
22	16.727	2449	2455	2467	rVB2	83661	165806	5.27%	0.796%
23	17.027	2501	2506	2511	rBV2	38564	76225	2.42%	0.366%
24	17.262	2534	2546	2555	rBV2	35573	132389	4.21%	0.636%
25	18.009	2666	2673	2678	rVB10	23638	52598	1.67%	0.252%
26	18.156	2690	2698	2706	rBV5	32841	88464	2.81%	0.425%
27	18.521	2754	2760	2775	rVB5	44543	151699	4.82%	0.728%

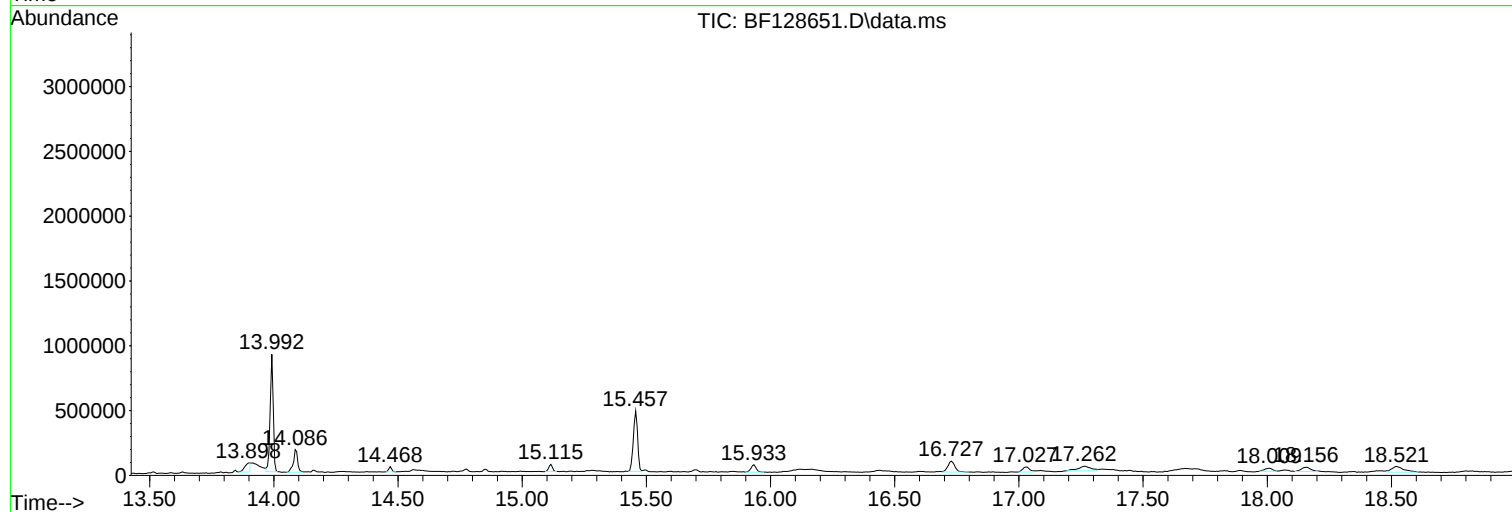
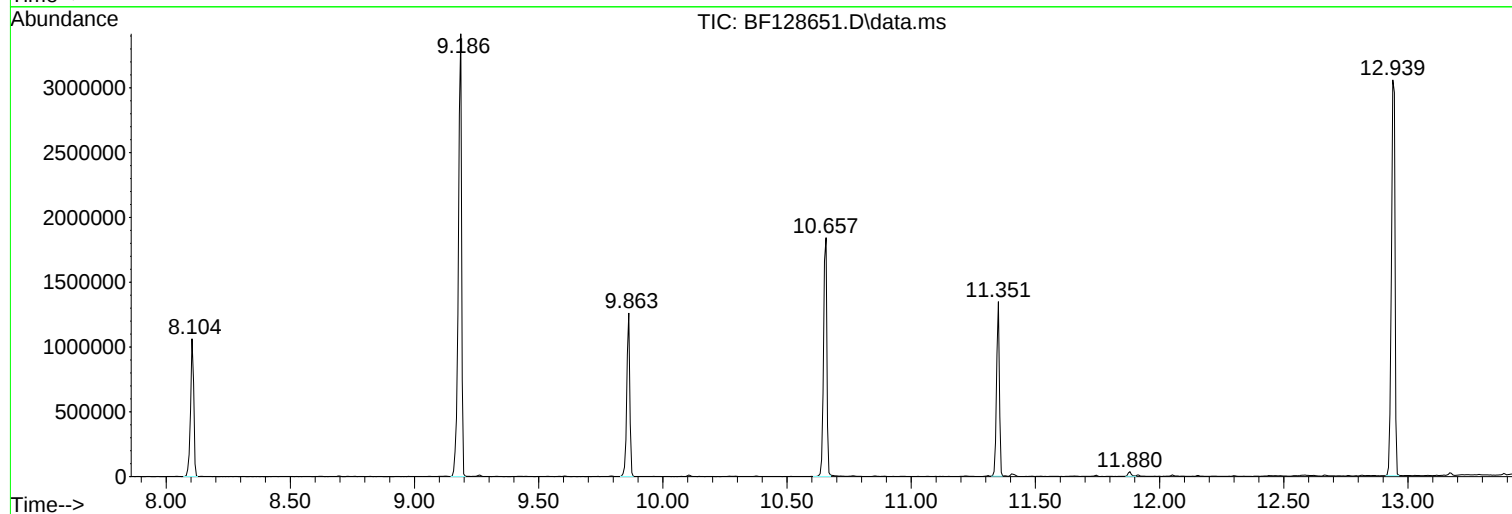
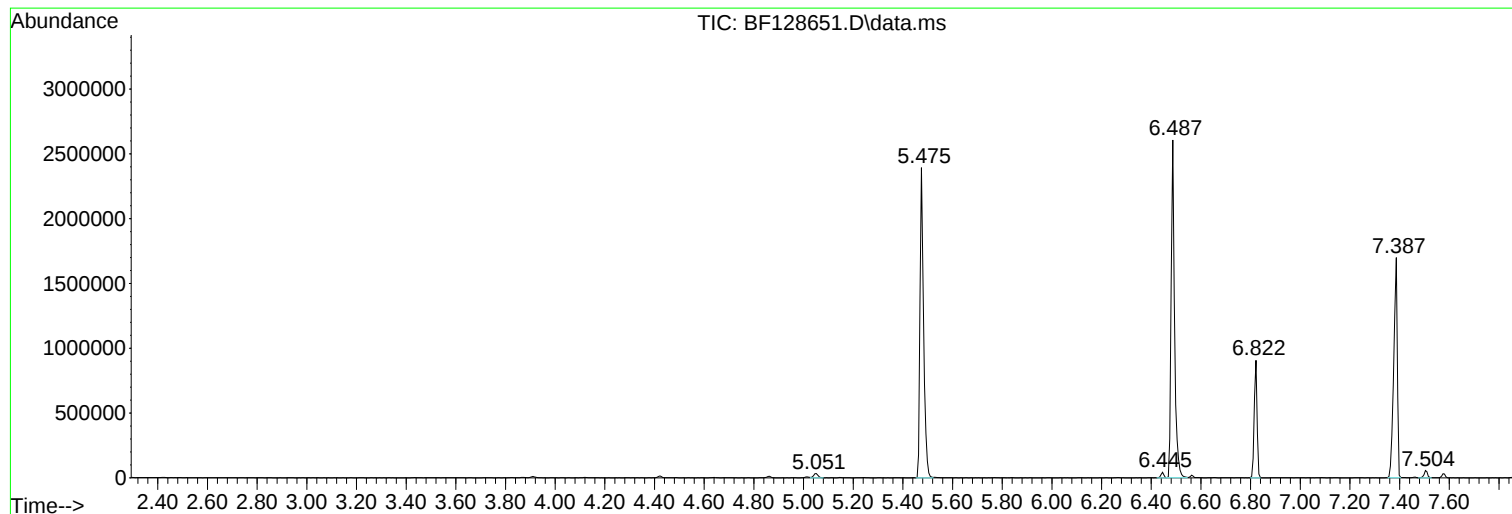
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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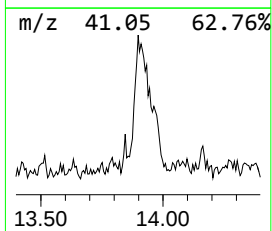
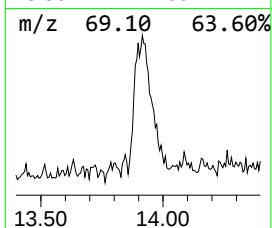
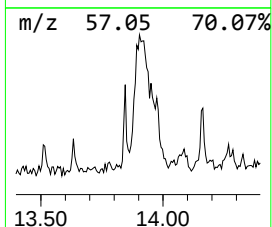
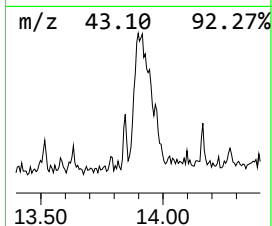
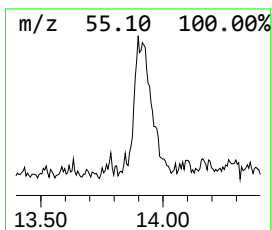
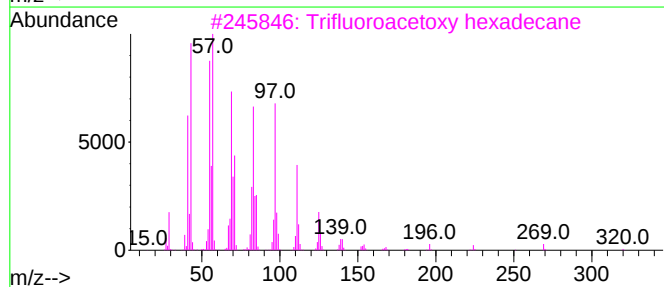
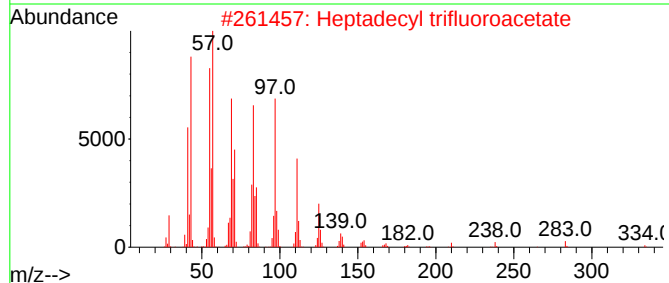
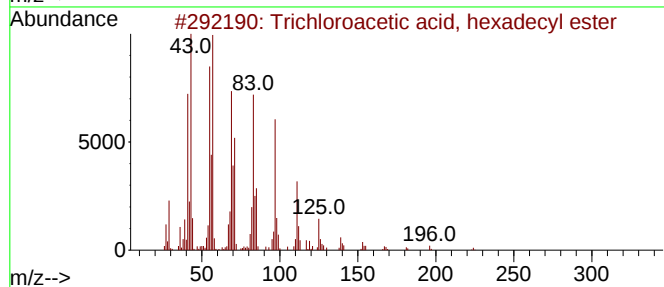
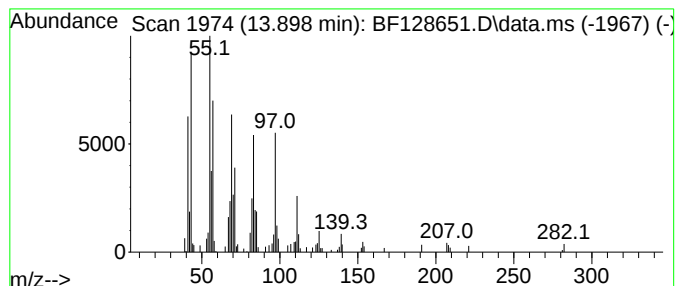
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.84 ng	112087	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4			1-Tetracosene	336	C24H48	010192-32-2	90
5			1-Docosene	308	C22H44	001599-67-3	90



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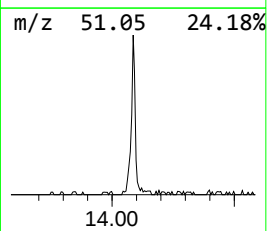
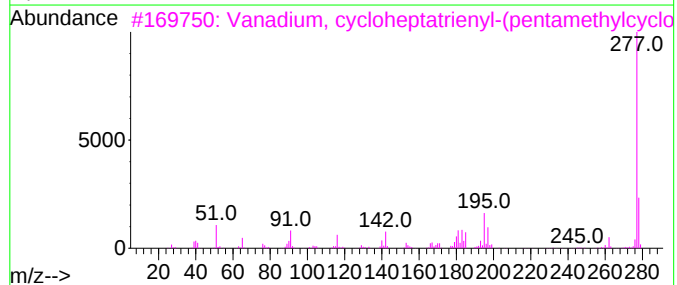
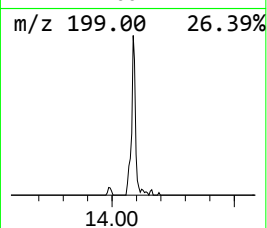
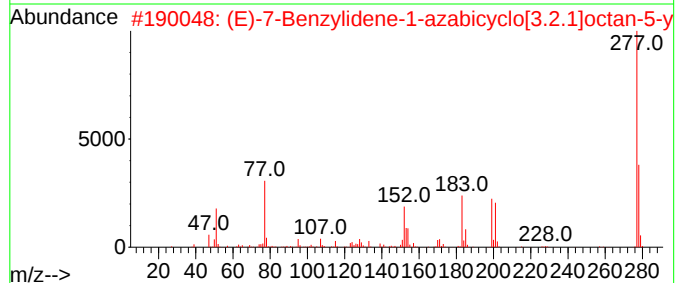
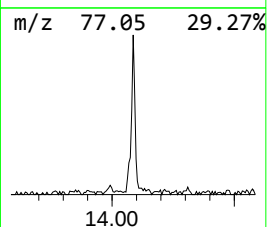
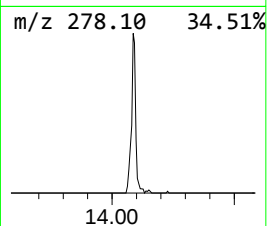
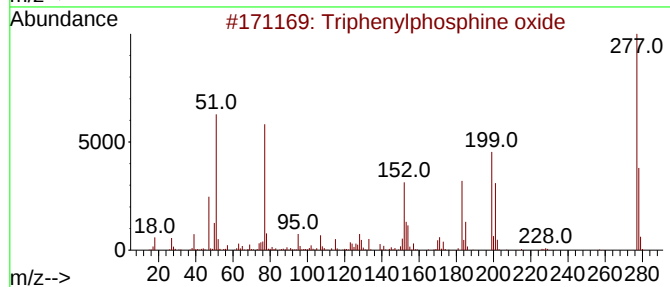
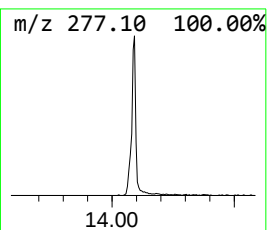
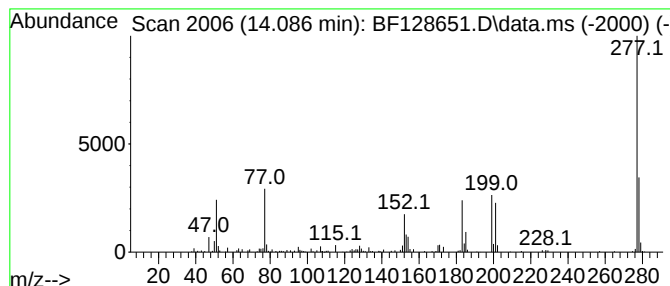
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	5.26 ng	207544	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	58
3			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
4			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	35



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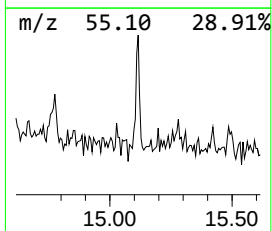
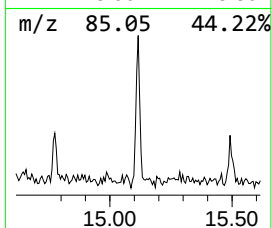
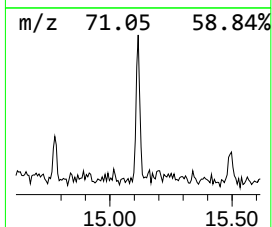
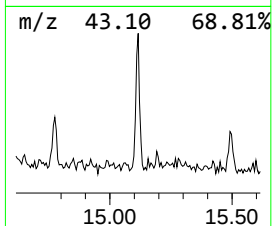
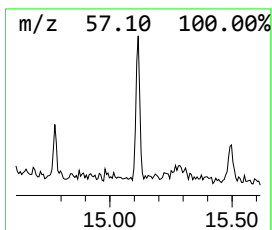
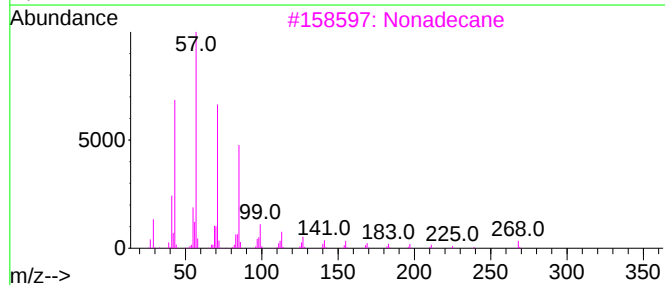
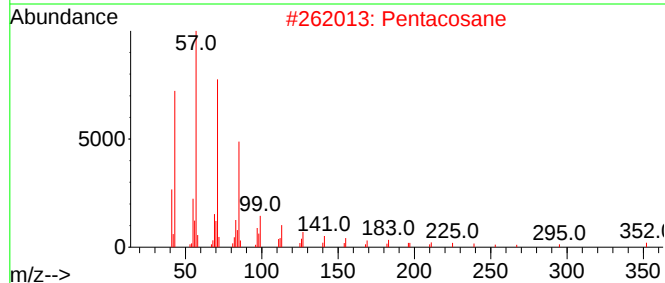
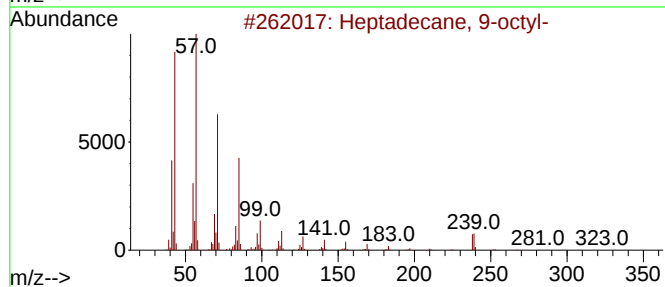
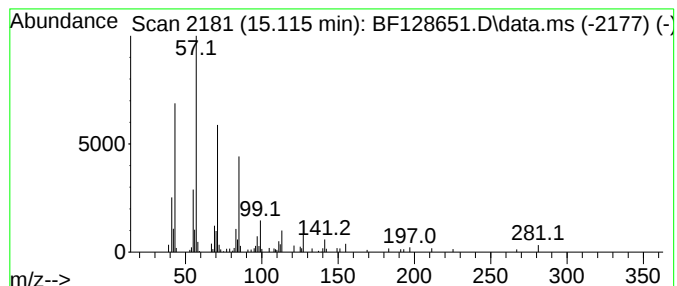
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.116	2.11 ng	59059	Perylene-d12	15.457

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Pentacosane	352	C25H52	000629-99-2	91
3		Nonadecane	268	C19H40	000629-92-5	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Hentriacontane	437	C31H64	000630-04-6	91



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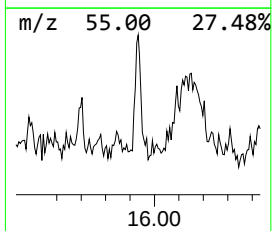
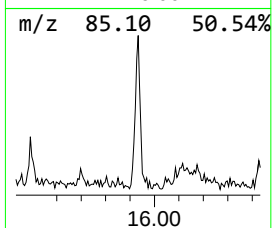
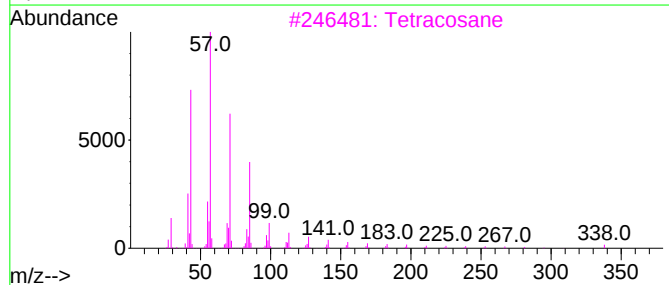
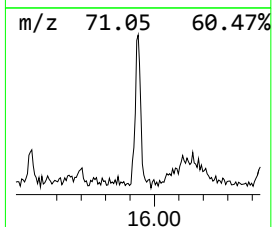
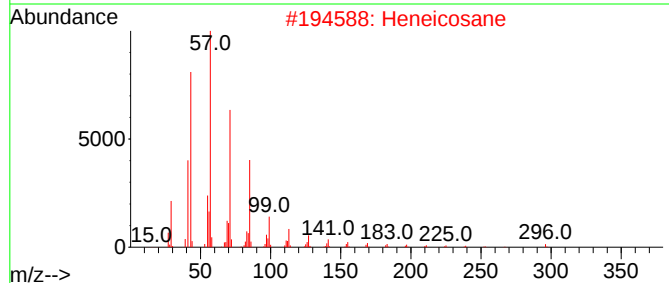
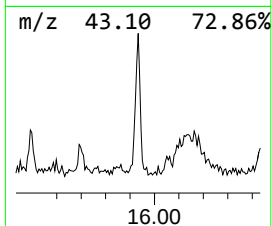
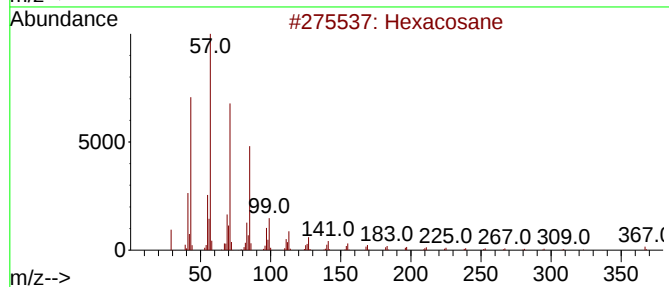
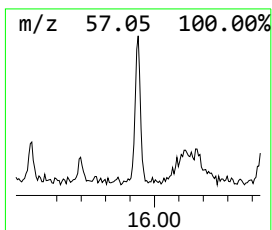
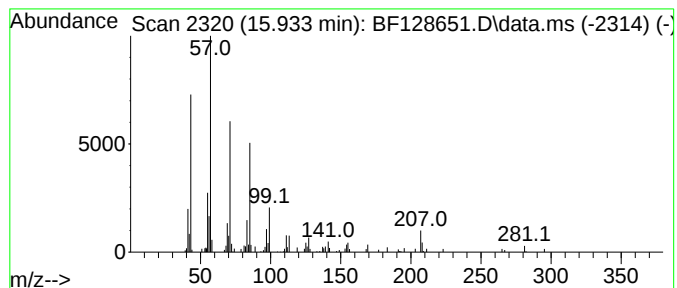
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.933	3.16 ng	88307	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	64
2			Heneicosane	296	C21H44	000629-94-7	64
3			Tetracosane	338	C24H50	000646-31-1	64
4			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	58
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	58



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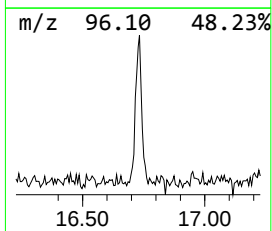
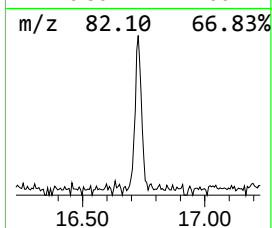
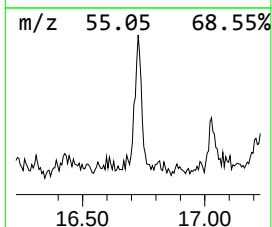
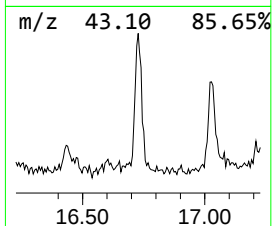
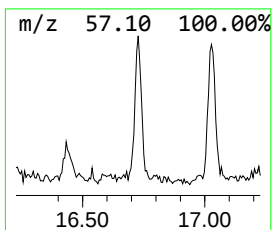
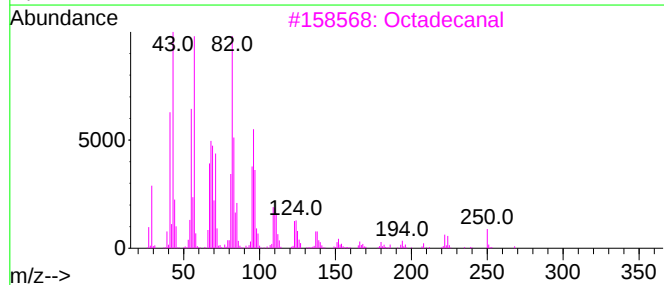
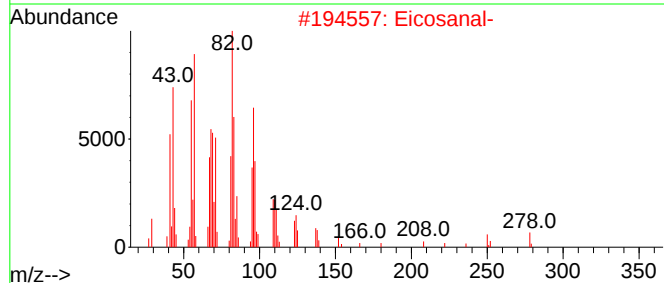
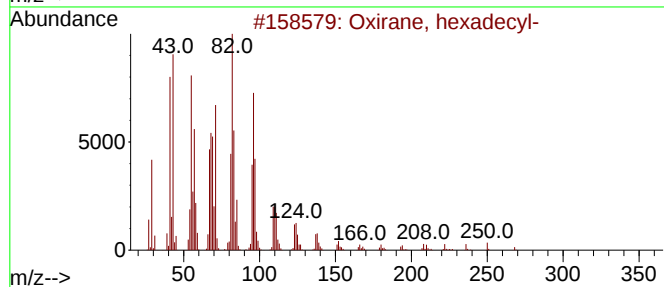
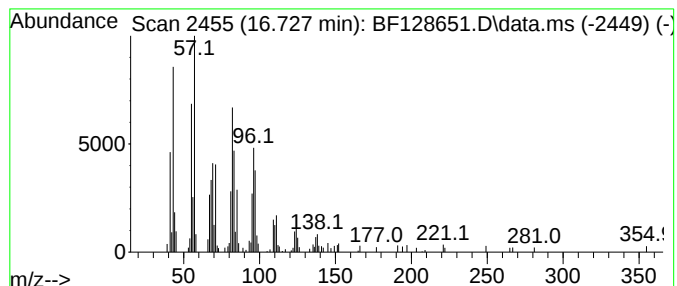
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Oxirane, hexadecyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.727	5.93 ng	165806	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2			Eicosanal-	296	C20H40O	002400-66-0	91
3			Octadecanal	268	C18H36O	000638-66-4	91
4			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
5			Tetracosanal	352	C24H48O	057866-08-7	90



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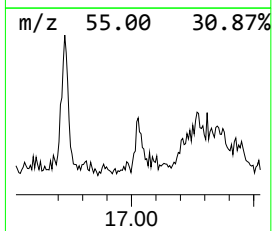
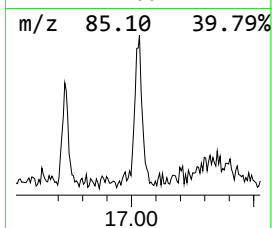
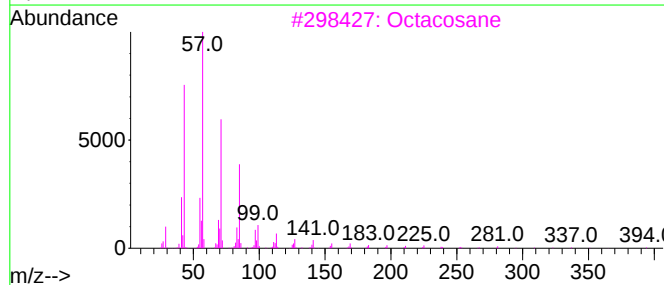
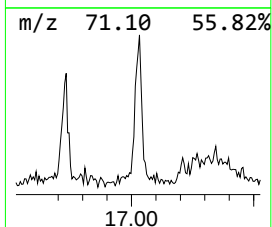
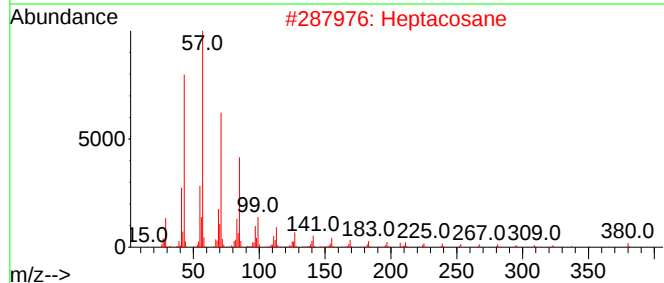
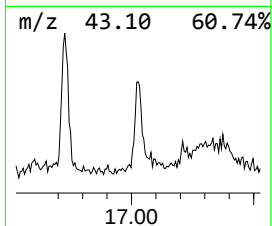
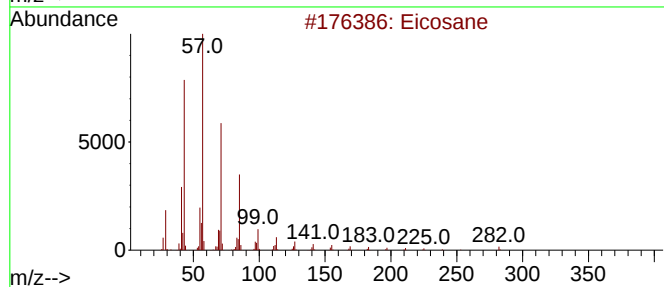
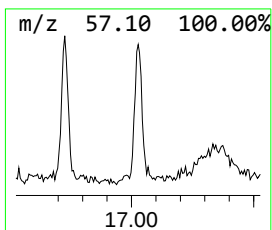
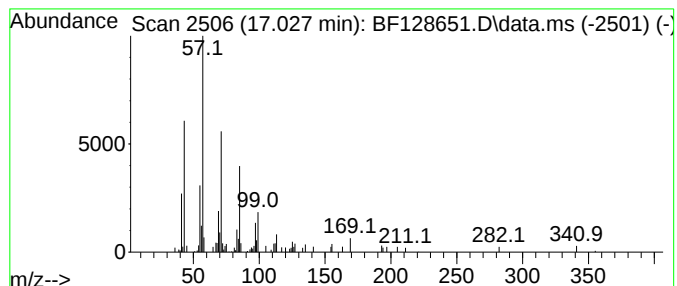
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.027	2.72 ng	76225	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	87
2	Heptacosane			380	C27H56	000593-49-7	87
3	Octacosane			394	C28H58	000630-02-4	86
4	Octadecane			254	C18H38	000593-45-3	86
5	Hexacosane			366	C26H54	000630-01-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060222\
Data File : BF128651.D
Acq On : 02 Jun 2022 21:40
Operator : CG\JU
Sample : N2988-24
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P015-SS006-0006-01

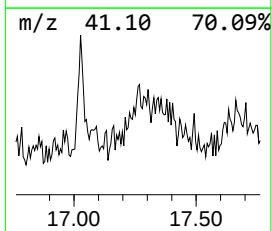
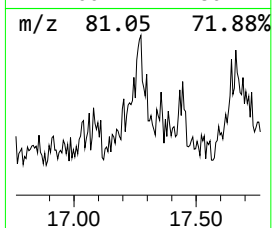
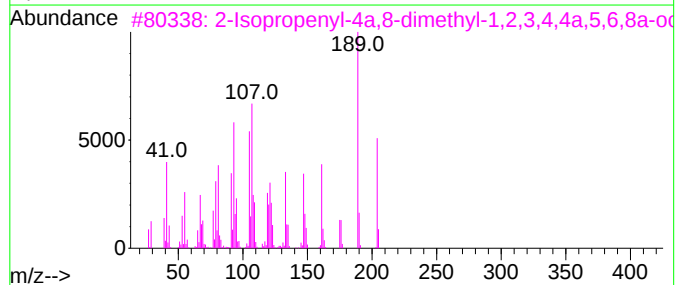
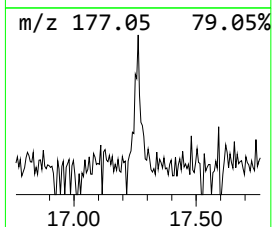
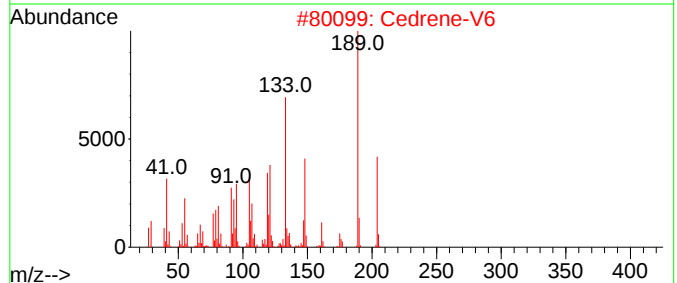
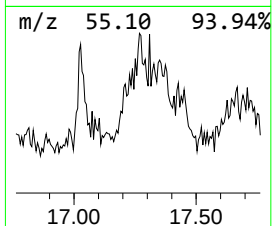
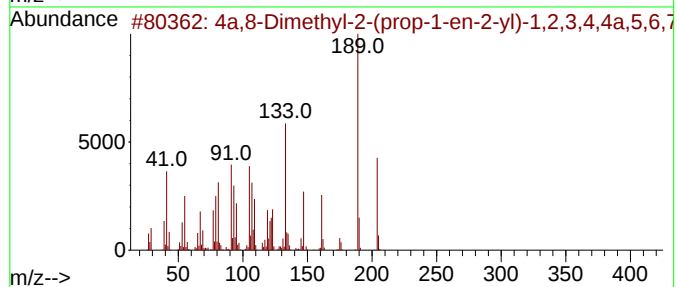
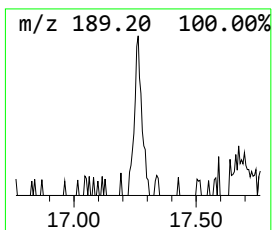
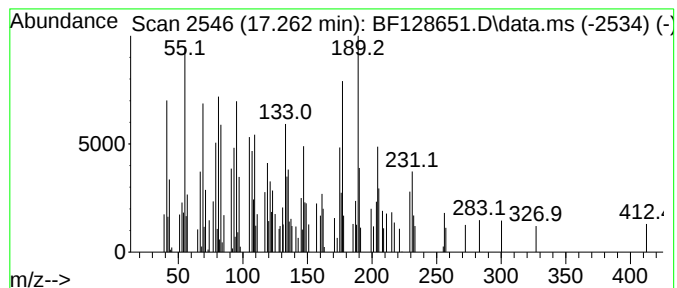
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.262 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.262	4.73 ng	132389	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	46		
2	Cedrene-V6	204	C15H24	1000162-76-8	42		
3	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	42		
4	2,6,10,10-Tetramethylbicyclo[7.2...	204	C15H24	136296-37-2	38		
5	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060222\
Data File : BF128651.D
Acq On : 02 Jun 2022 21:40
Operator : CG\JU
Sample : N2988-24
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P015-SS006-0006-01

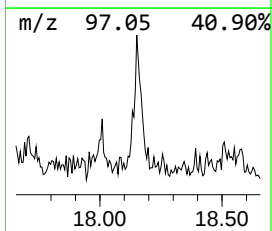
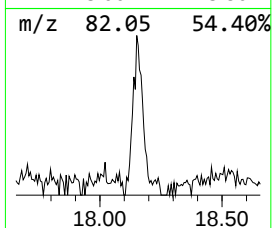
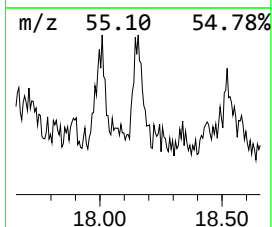
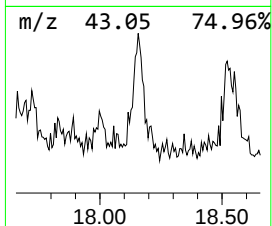
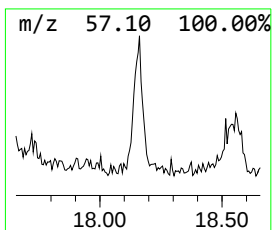
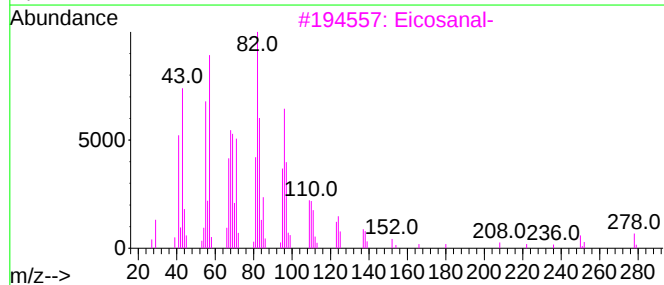
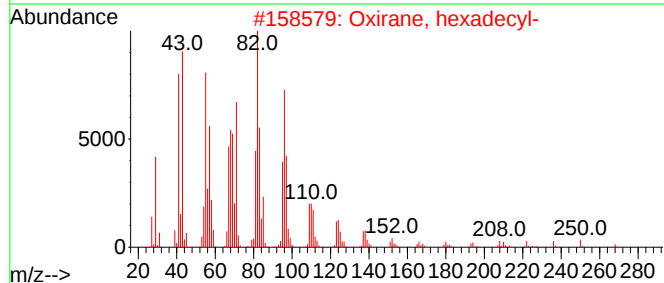
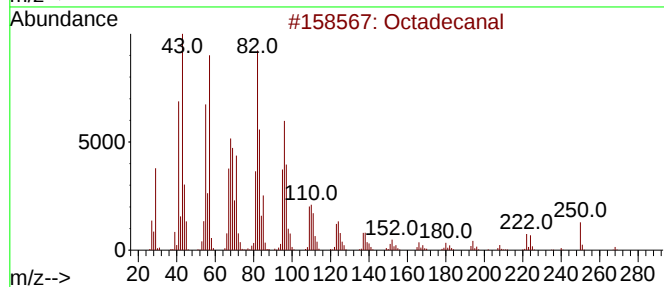
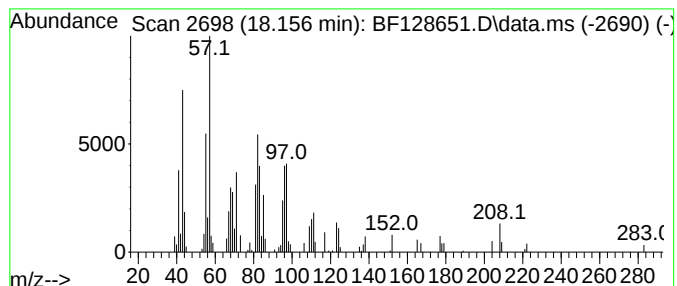
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	3.16 ng	88464	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	74
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	72
3			Eicosanal-	296	C20H40O	002400-66-0	64
4			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	62
5			9-Octadecen-1-ol, (Z)-	268	C18H36O	000143-28-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060222\
Data File : BF128651.D
Acq On : 02 Jun 2022 21:40
Operator : CG\JU
Sample : N2988-24
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P015-SS006-0006-01

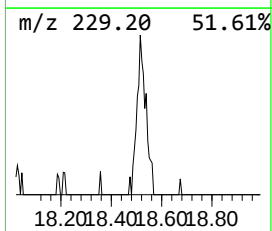
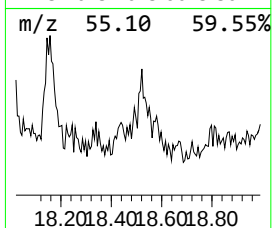
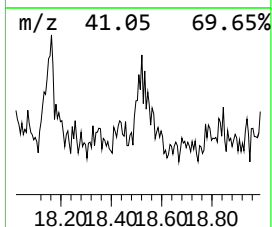
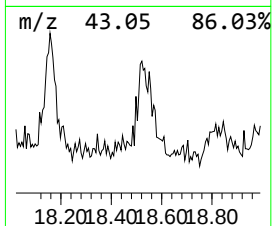
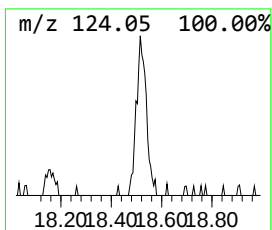
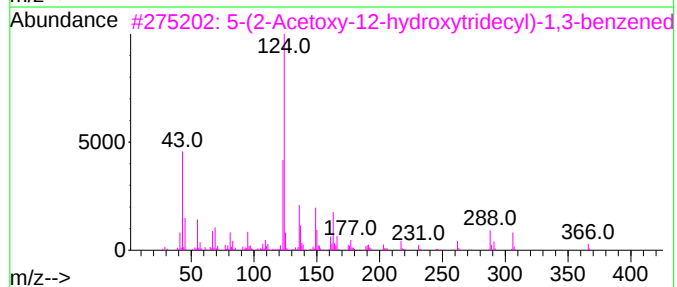
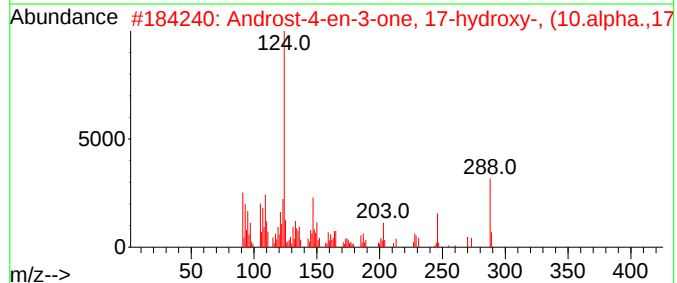
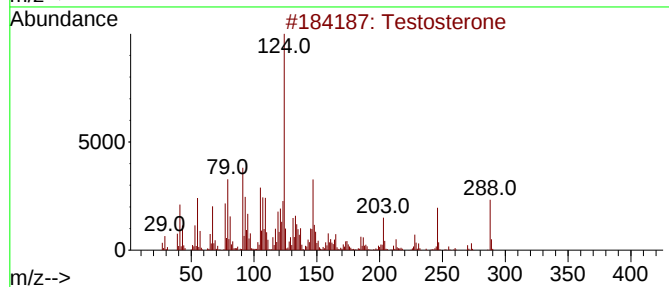
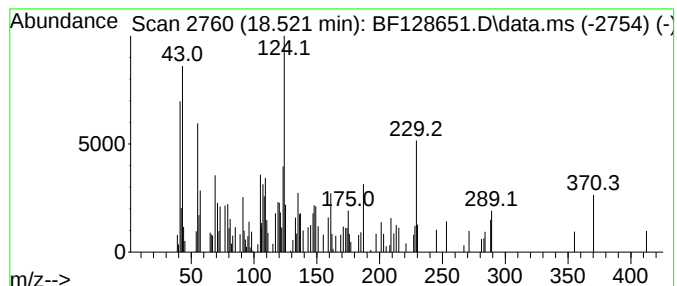
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown18.521 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.521	5.42 ng	151699	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Testosterone	288	C19H28O2	000058-22-0	46
2			Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000604-39-7	46
3			5-(2-Acetoxy-12-hydroxytridecyl)...	366	C21H34O5	913690-44-5	38
4			1,3-Benzenediol, 2-methyl-	124	C7H8O2	000608-25-3	35
5			2,4-Diaminophenol	124	C6H8N2O	000095-86-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060222\
Data File : BF128651.D
Acq On : 02 Jun 2022 21:40
Operator : CG\JU
Sample : N2988-24
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P015-SS006-0006-01

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
Trichloroacetic...	13.898	2.8	ng	112087	5	13.992	788421	20.0
Triphenylphosph...	14.086	5.3	ng	207544	5	13.992	788421	20.0
Heptadecane, 9-...	15.116	2.1	ng	59059	6	15.457	559673	20.0
Hexacosane	15.933	3.2	ng	88307	6	15.457	559673	20.0
Oxirane, hexade...	16.727	5.9	ng	165806	6	15.457	559673	20.0
Eicosane	17.027	2.7	ng	76225	6	15.457	559673	20.0
unknown17.262	17.262	4.7	ng	132389	6	15.457	559673	20.0
Octadecanal	18.157	3.2	ng	88464	6	15.457	559673	20.0
unknown18.521	18.521	5.4	ng	151699	6	15.457	559673	20.0