

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102120\
 Data File : BF122061.D
 Acq On : 21 Oct 2020 18:15
 Operator : JU/CG
 Sample : L4467-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-240

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-BF101220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122061.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.951	484	487	502	rVB	35824	55784	1.66%	0.239%
2	5.351	551	555	587	rBV	2734026	2869412	85.55%	12.277%
3	6.381	725	730	747	rBV	2545943	2965008	88.40%	12.686%
4	6.581	761	764	777	rBV	26847	54188	1.62%	0.232%
5	6.722	785	788	798	rVB	707541	646371	19.27%	2.766%
6	7.298	881	886	898	rBV	2058176	2035997	60.70%	8.711%
7	8.010	1003	1007	1023	rBV	913708	855602	25.51%	3.661%
8	9.080	1184	1189	1200	rBV	3382869	3354269	100.00%	14.351%
9	9.480	1253	1257	1265	rBV	421019	370563	11.05%	1.585%
10	9.757	1300	1304	1315	rVB	1111376	970590	28.94%	4.153%
11	10.551	1435	1439	1455	rBV	2277947	2136826	63.70%	9.142%
12	11.239	1553	1556	1560	rBV	987163	963054	28.71%	4.120%
13	11.774	1644	1647	1650	rBV2	68643	67945	2.03%	0.291%
14	12.457	1759	1763	1768	rVB	101889	92384	2.75%	0.395%
15	12.680	1797	1801	1806	rVB	78034	85027	2.53%	0.364%
16	12.827	1821	1826	1829	rBV	3392811	3150425	93.92%	13.479%
17	13.727	1974	1979	1991	rBV	224068	468298	13.96%	2.004%
18	13.880	2001	2005	2008	rBV	752581	689869	20.57%	2.952%
19	14.110	2041	2044	2048	rBV	41661	58692	1.75%	0.251%
20	14.333	2079	2082	2085	rBV2	29366	36690	1.09%	0.157%
21	14.368	2085	2088	2100	rVV10	26988	69103	2.06%	0.296%
22	14.498	2105	2110	2111	rBV5	41411	59915	1.79%	0.256%
23	14.774	2152	2157	2170	rVB2	51677	170511	5.08%	0.730%
24	14.904	2175	2179	2182	rBV	51270	81017	2.42%	0.347%
25	14.951	2184	2187	2193	rVB3	61567	93735	2.79%	0.401%
26	15.251	2235	2238	2242	rVB	35160	44406	1.32%	0.190%
27	15.309	2243	2248	2259	rVB	547184	699880	20.87%	2.994%
28	15.715	2312	2317	2322	rVB3	42955	67993	2.03%	0.291%
29	15.804	2326	2332	2338	rBV9	45176	118933	3.55%	0.509%
30	16.721	2484	2488	2495	rVB4	20572	40032	1.19%	0.171%

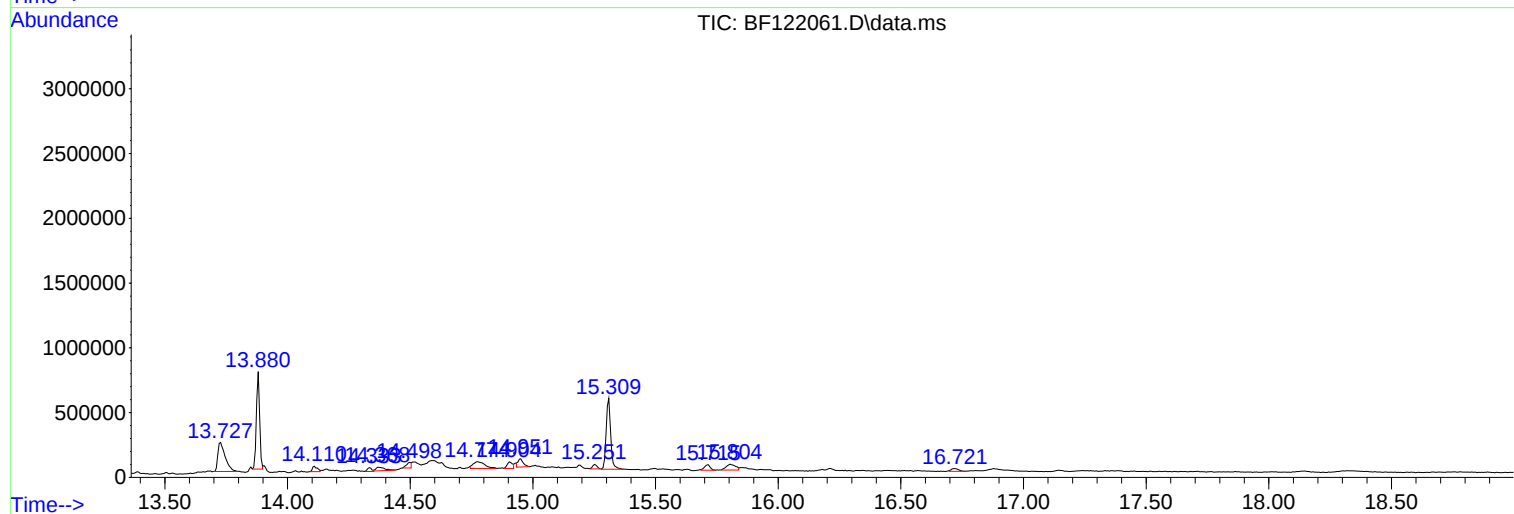
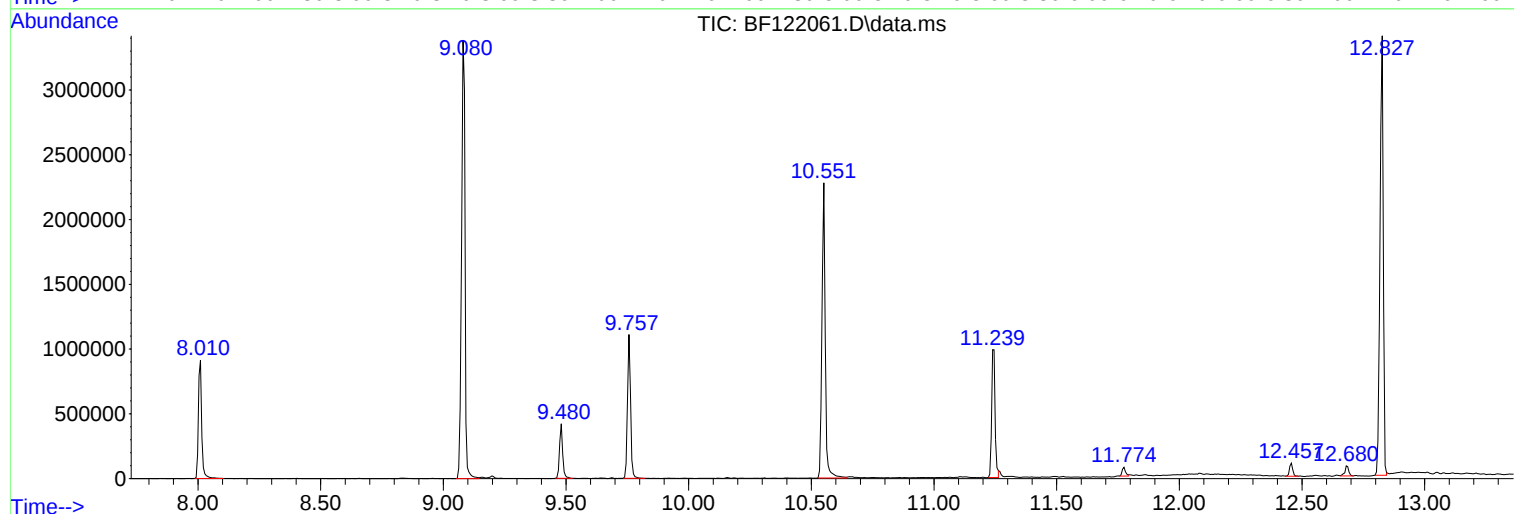
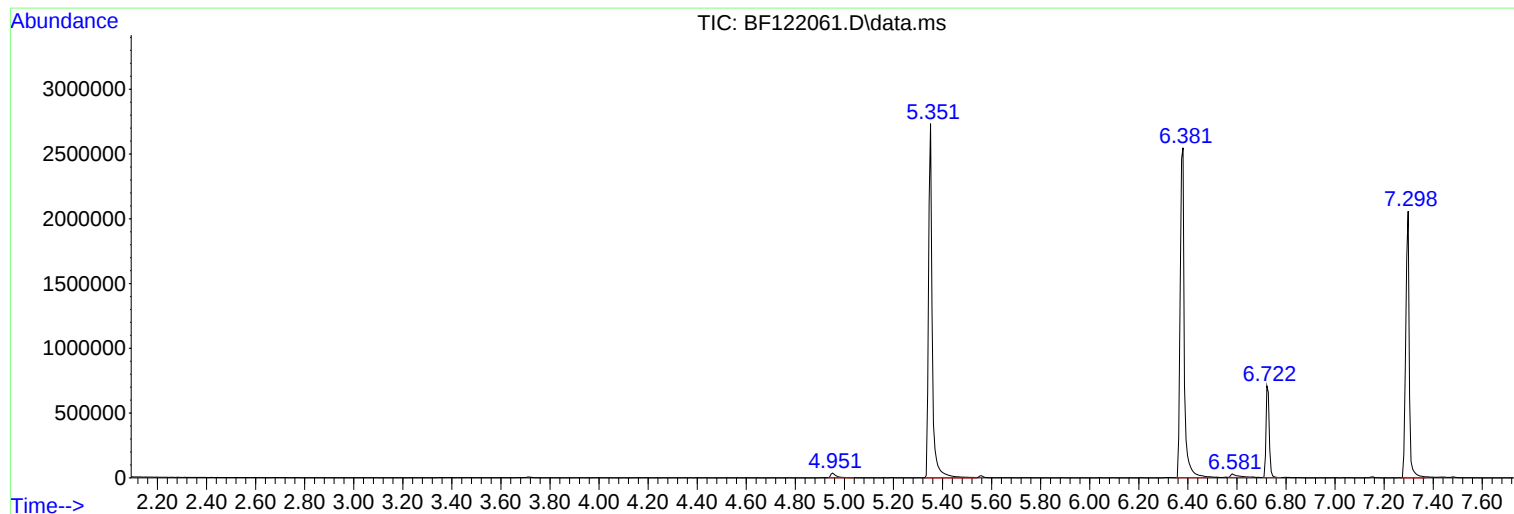
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Instrument :
BNA_F
ClientSampleId :
VNJ-240

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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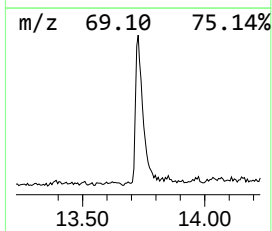
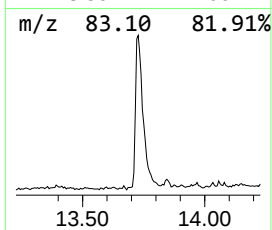
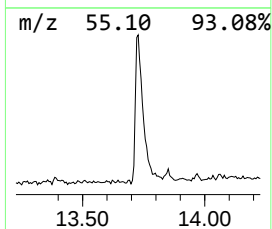
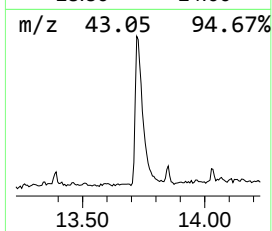
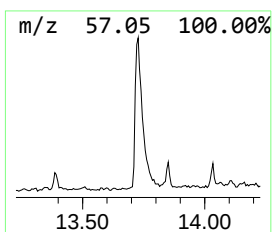
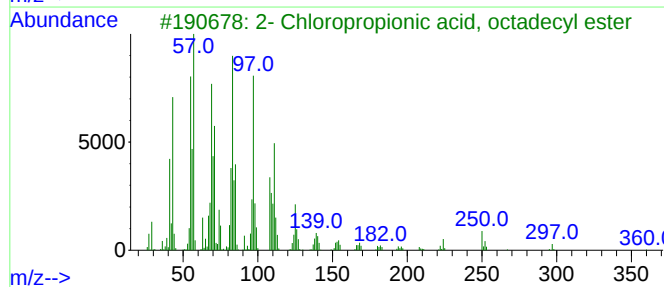
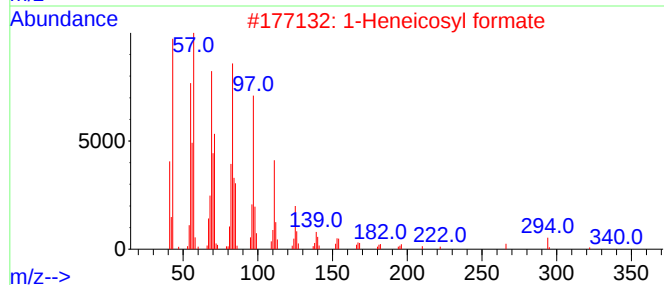
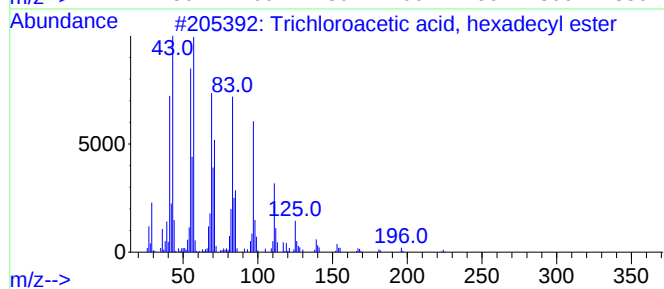
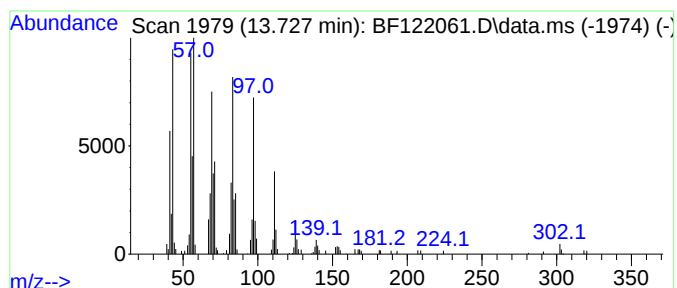
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Trichloroacetic acid, hexadecyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	13.58 ng	468298	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94



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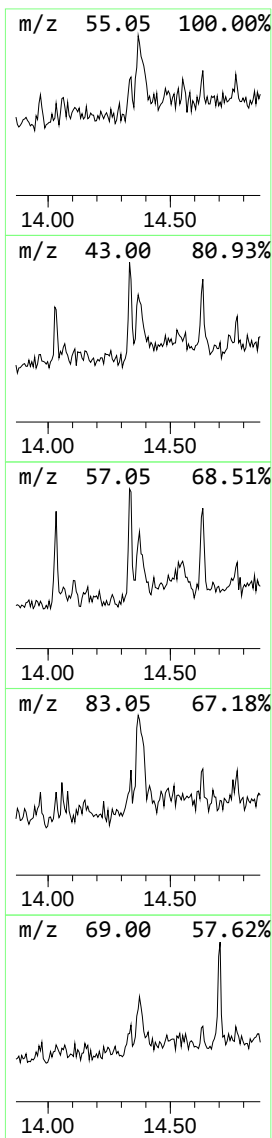
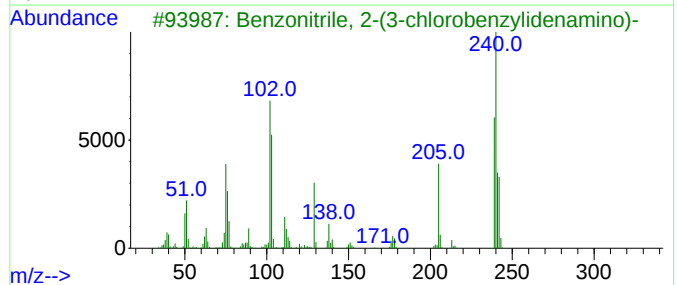
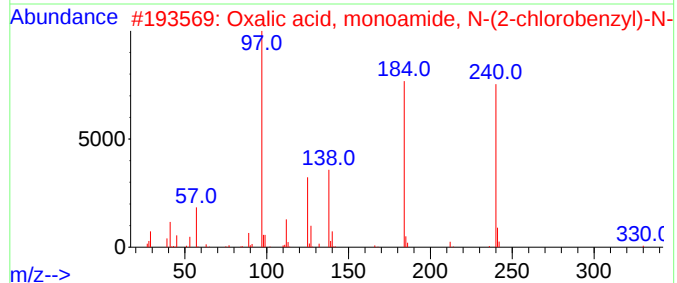
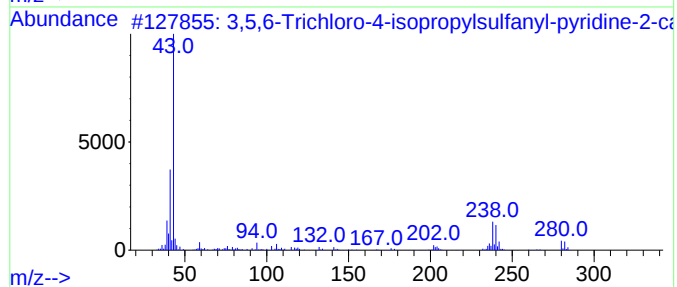
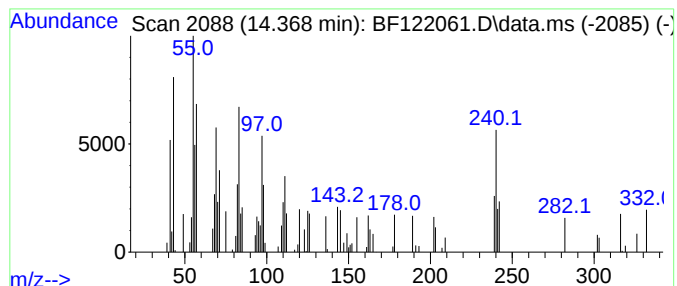
Instrument :
BNA_F
ClientSampleId :
VNJ-240

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown14.36 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.368	2.00 ng	69103	Chrysene-d12	13.880		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5,6-Trichloro-4-isopropylsulfa...	280	C9H7Cl3N2S	216242-35-2	22	
2	Oxalic acid, monoamide, N-(2-chl...	365	C18H20ClN03S	1000309-74-3	16	
3	Benzonitrile, 2-(3-chlorobenzylid...	240	C14H9ClN2	315670-35-0	12	
4	p-Bromophenyl trifluoromethyl ether	240	C7H4BrF3O	000407-14-7	12	
5	Diisopropylketone p-tosylhydrazone	282	C14H22N2O2S	017530-00-6	10	



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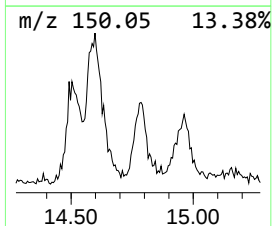
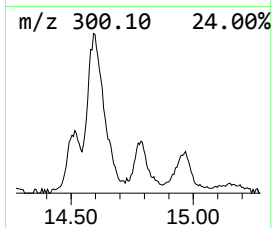
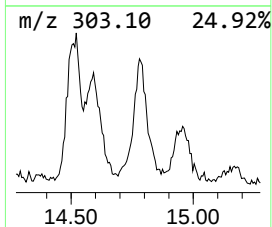
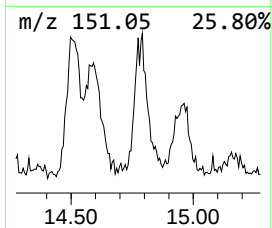
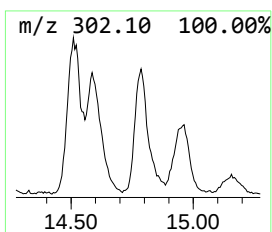
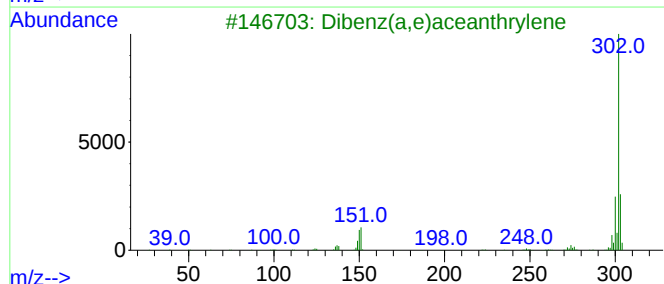
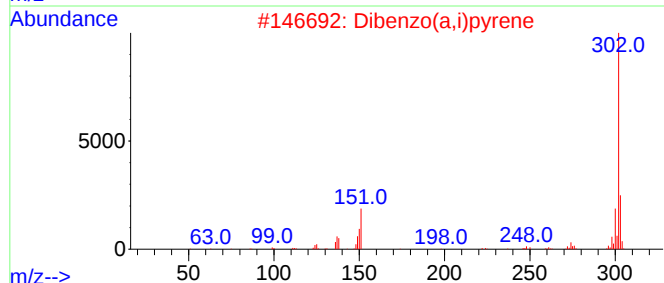
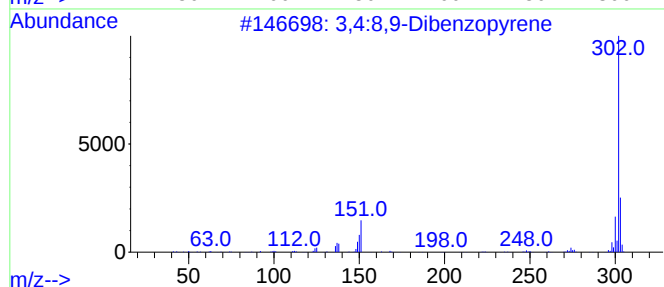
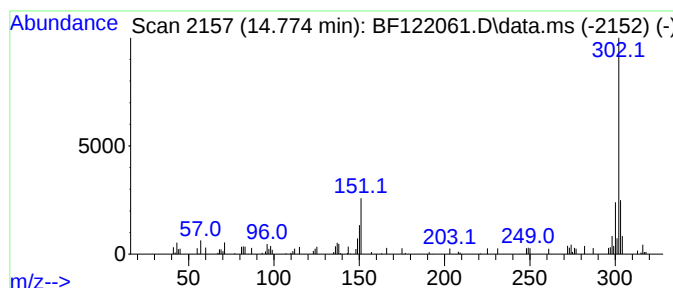
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3,4:8,9-Dibenzopyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.774	4.87 ng	170511	Perylene-d12	15.310	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	96
2	Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	95
3	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	76
4	1,2,9,10-Dibenzopyrene	302	C24H14	000191-30-0	76
5	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	72



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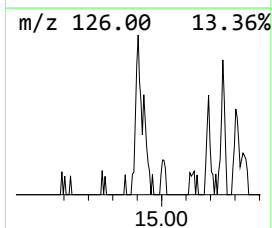
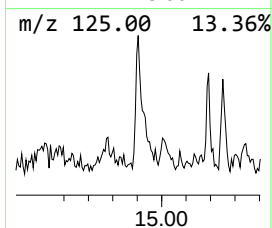
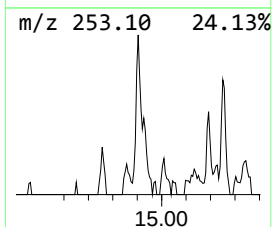
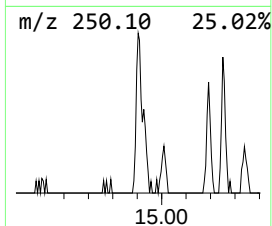
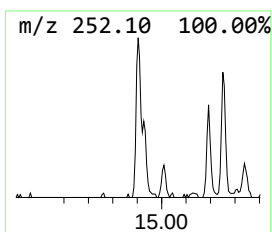
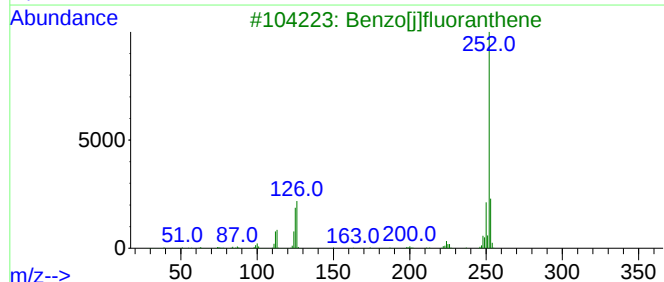
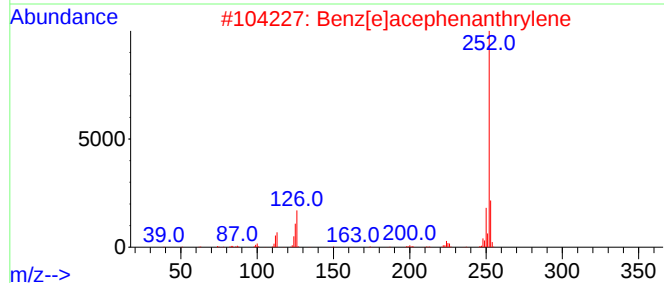
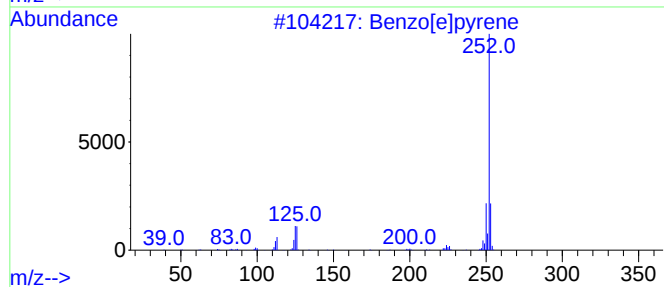
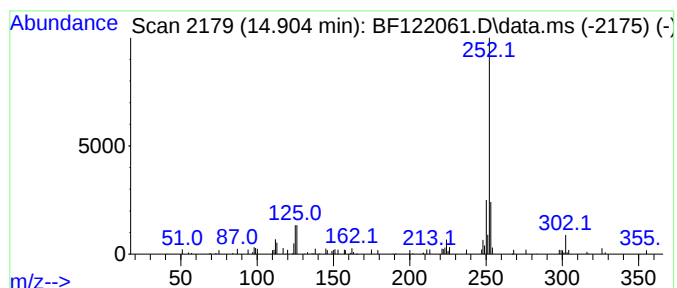
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	2.32 ng	81017	Perylene-d12	15.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4			Perylene	252	C20H12	000198-55-0	93
5			Benzo[a]pyrene	252	C20H12	000050-32-8	89



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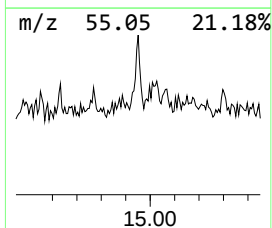
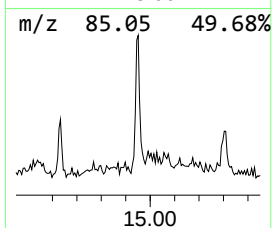
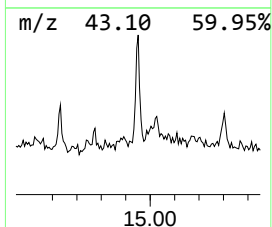
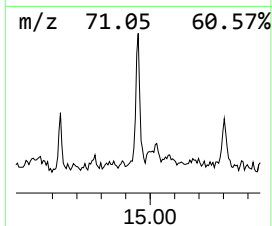
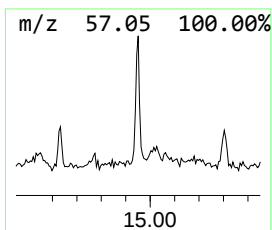
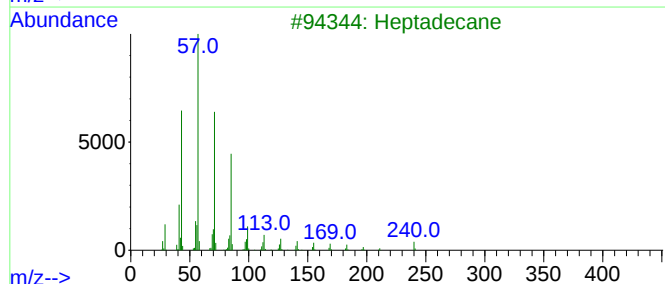
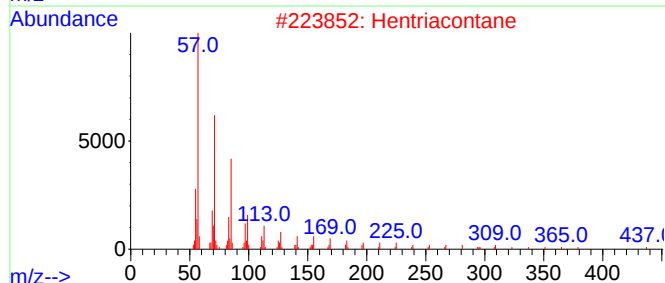
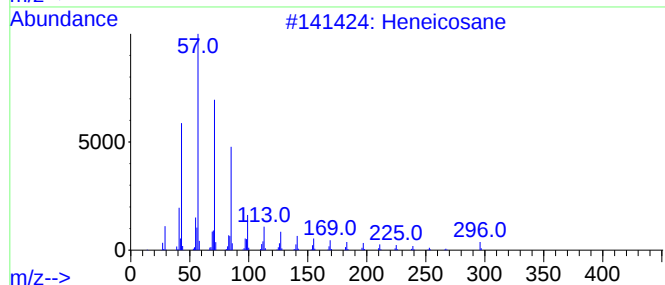
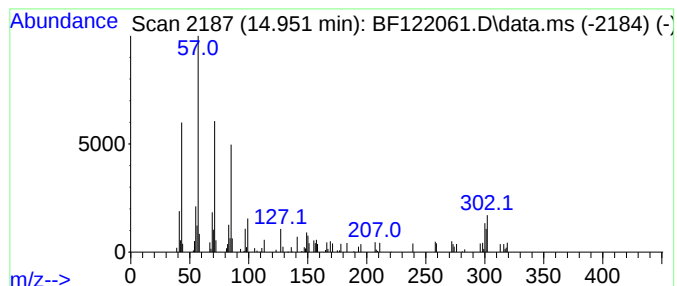
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.951	2.68 ng	93735	Perylene-d12	15.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Hentriacontane	437	C31H64	000630-04-6	53
3			Heptadecane	240	C17H36	000629-78-7	49
4			Pentacosane	352	C25H52	000629-99-2	49
5			Octacosane	394	C28H58	000630-02-4	49



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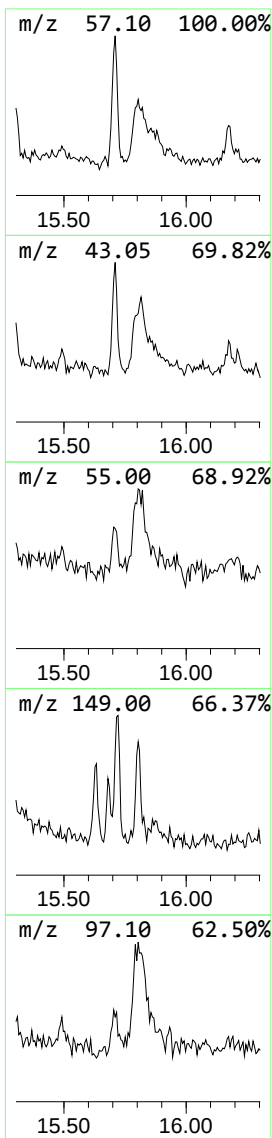
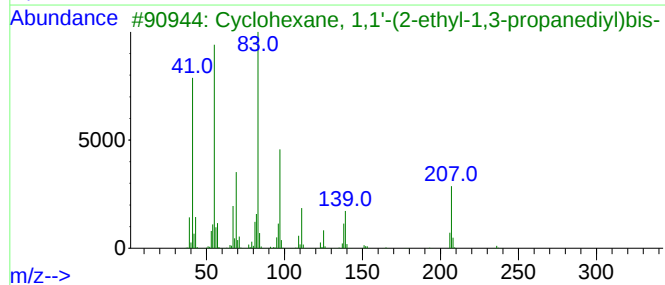
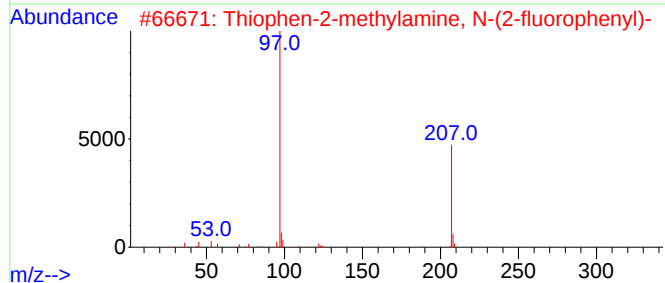
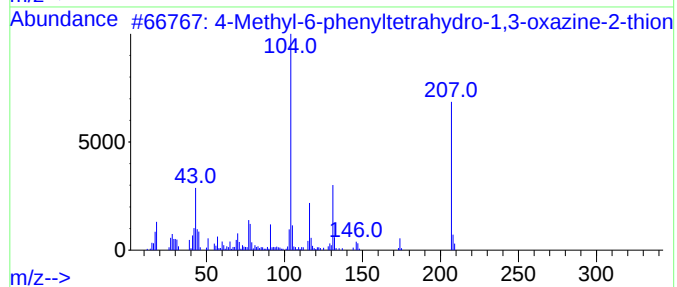
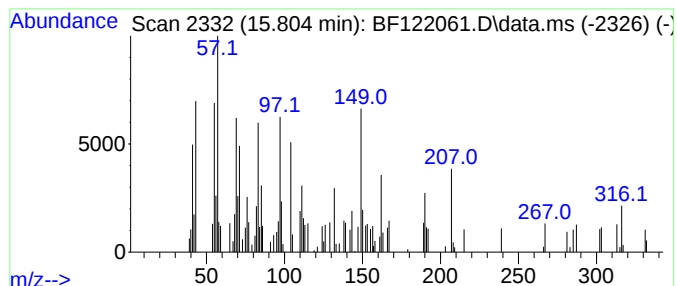
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.80 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.804	3.40 ng	118933	Perylene-d12	15.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-6-phenyltetrahydro-1,3-...	207	C11H13NOS	086071-94-5	25		
2	Thiophen-2-methylamine, N-(2-flu...	207	C11H10FNS	1000310-35-2	22		
3	Cyclohexane, 1,1'-(2-ethyl-1,3-p...	236	C17H32	054833-34-0	22		
4	Phthalic acid, 2-bromo-4-fluorop...	434	C21H20BrFO4	1000315-62-9	12		
5	Phthalic acid, 2-chloropropyl he...	466	C27H43ClO4	1000356-83-7	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102120\
Data File : BF122061.D
Acq On : 21 Oct 2020 18:15
Operator : JU/CG
Sample : L4467-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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
Trichloroacetic...	13.727	13.6	ng	468298	5	13.880	689869	20.0
unknown14.36	14.368	2.0	ng	69103	5	13.880	689869	20.0
3,4:8,9-Dibenzo...	14.774	4.9	ng	170511	6	15.310	699880	20.0
Benzo[e]pyrene	14.904	2.3	ng	81017	6	15.310	699880	20.0
Heneicosane	14.951	2.7	ng	93735	6	15.310	699880	20.0
unknown15.80	15.804	3.4	ng	118933	6	15.310	699880	20.0