

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051921\
 Data File : BF123993.D
 Acq On : 19 May 2021 16:41
 Operator : JU/CG
 Sample : M2439-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-72-11939

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-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123993.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	8	13	18	rVB	457728	553750	50.46%	5.982%
2	2.275	27	32	40	rVB	30628	41522	3.78%	0.449%
3	5.116	507	515	520	rBV	58351	79594	7.25%	0.860%
4	5.516	578	583	586	rBV	1074225	930006	84.75%	10.046%
5	6.522	749	754	757	rBV	1083365	959352	87.42%	10.363%
6	6.728	785	789	795	rBV	40792	37103	3.38%	0.401%
7	6.904	816	819	822	rBV	363440	273116	24.89%	2.950%
8	7.463	910	914	917	rBV	816492	632834	57.67%	6.836%
9	8.186	1033	1037	1040	rBV	469425	355645	32.41%	3.842%
10	9.263	1216	1220	1223	rBV	1496738	1097405	100.00%	11.854%
11	9.375	1235	1239	1242	rBV	115409	99602	9.08%	1.076%
12	9.651	1283	1286	1292	rBV	165904	131039	11.94%	1.416%
13	9.945	1332	1336	1339	rBV	457057	410257	37.38%	4.432%
14	10.727	1465	1469	1477	rBV	887716	732846	66.78%	7.916%
15	11.427	1585	1588	1591	rBV	475594	395021	36.00%	4.267%
16	11.451	1591	1592	1595	rVB	48369	26519	2.42%	0.286%
17	11.951	1674	1677	1680	rBV2	40706	36510	3.33%	0.394%
18	12.639	1791	1794	1798	rBV	87228	80494	7.33%	0.870%
19	12.868	1828	1833	1839	rVB	72183	76537	6.97%	0.827%
20	13.016	1854	1858	1861	rBV	1194703	942822	85.91%	10.185%
21	13.910	2007	2010	2019	rBV2	114303	124414	11.34%	1.344%
22	14.051	2029	2034	2036	rBV	308078	333378	30.38%	3.601%
23	14.068	2036	2037	2040	rVV	355771	246629	22.47%	2.664%
24	14.092	2040	2041	2048	rVB	42420	38904	3.55%	0.420%
25	14.545	2115	2118	2122	rBV5	21856	26283	2.40%	0.284%
26	14.704	2141	2145	2148	rBV3	22471	22824	2.08%	0.247%
27	15.004	2193	2196	2200	rVB5	20851	22018	2.01%	0.238%
28	15.121	2212	2216	2219	rBV	40264	55121	5.02%	0.595%
29	15.204	2227	2230	2233	rBV4	21713	22404	2.04%	0.242%
30	15.233	2233	2235	2241	rVB4	29037	34692	3.16%	0.375%
31	15.433	2266	2269	2273	rBV	24279	32739	2.98%	0.354%
32	15.498	2275	2280	2284	rVV3	25228	36675	3.34%	0.396%
33	15.562	2286	2291	2296	rVV	225334	290275	26.45%	3.136%
34	15.604	2296	2298	2303	rVB5	20772	25982	2.37%	0.281%
35	16.057	2371	2375	2379	rBV3	22854	31134	2.84%	0.336%
36	17.068	2541	2547	2552	rBV8	13048	21892	1.99%	0.236%

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ClientSampleId :
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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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

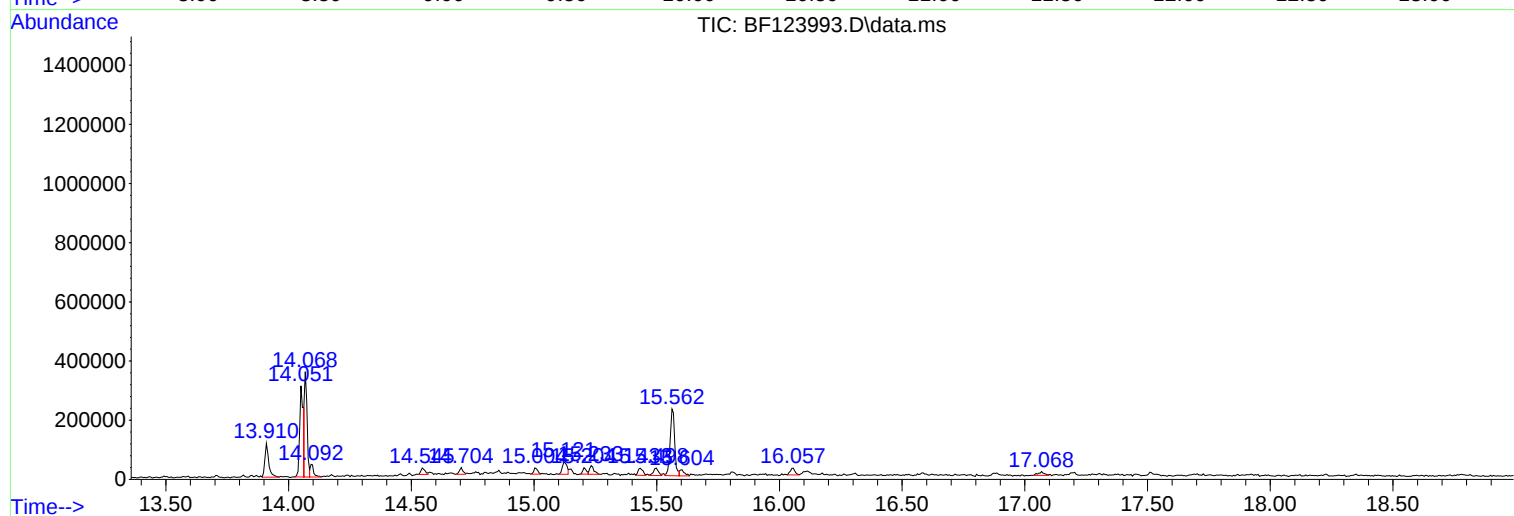
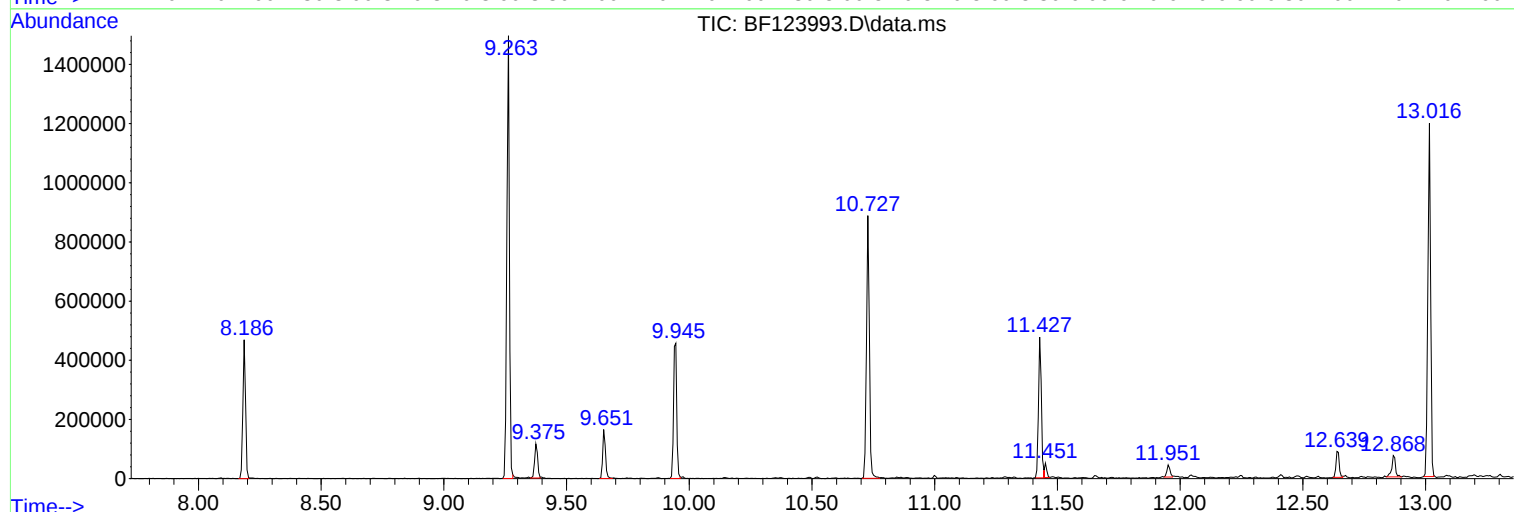
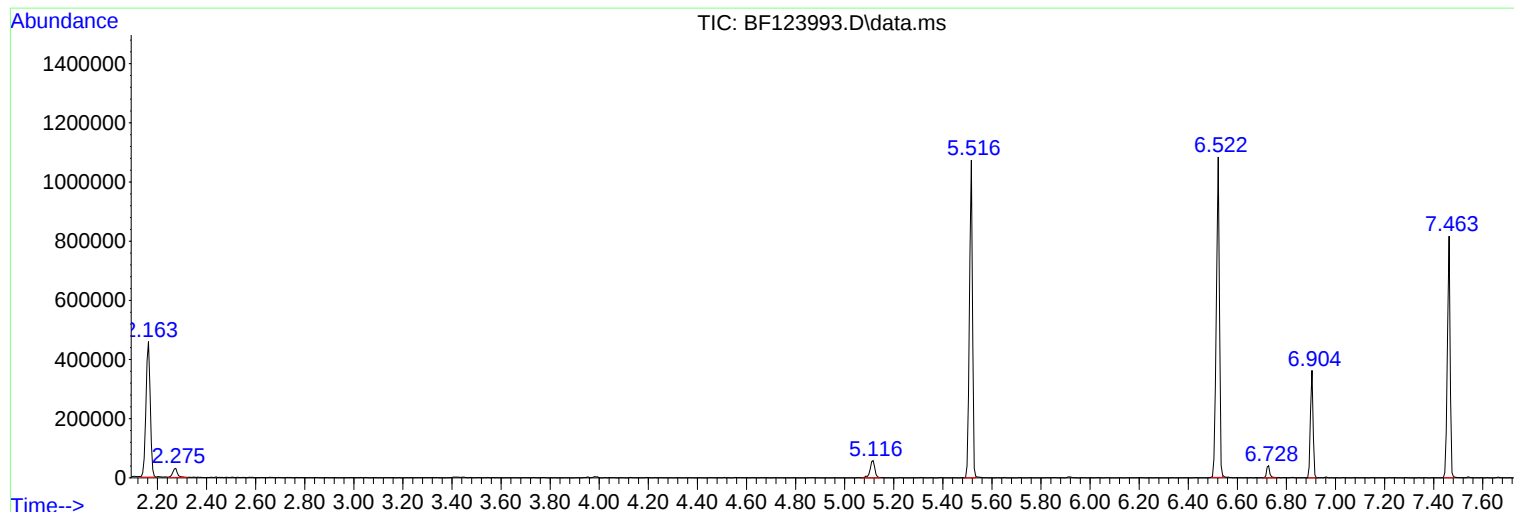
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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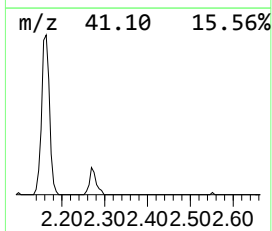
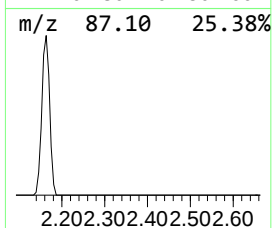
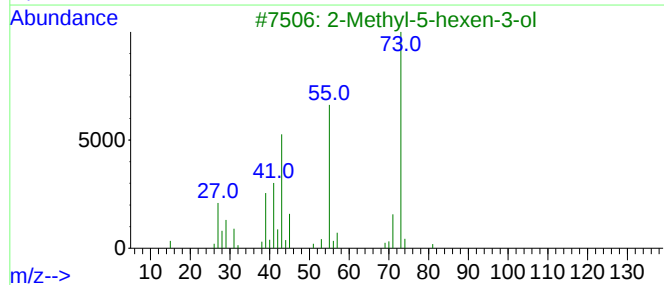
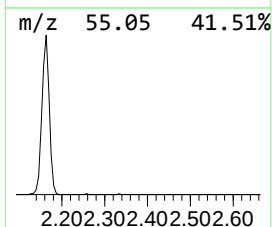
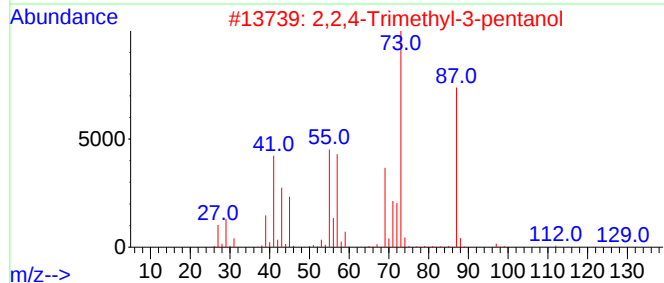
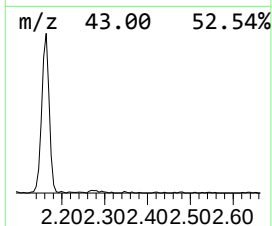
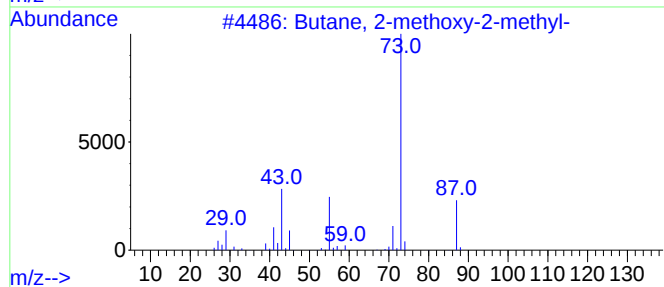
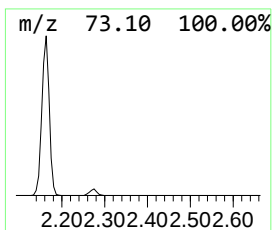
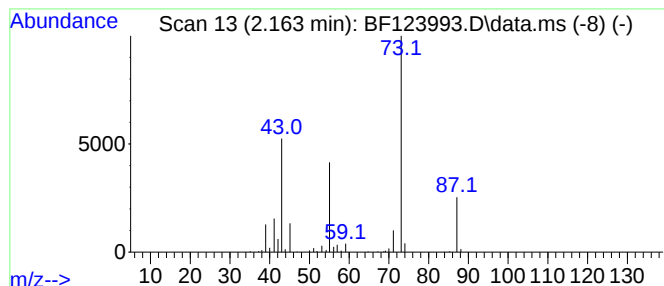
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	40.55 ng	553750	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
4			4-Penten-2-ol, acetate	128	C7H12O2	1000352-31-5	10
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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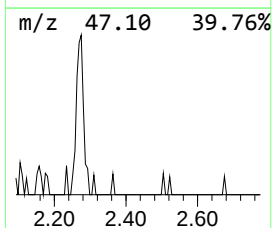
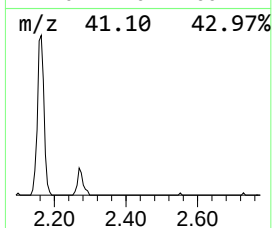
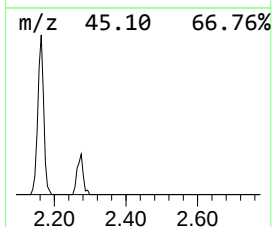
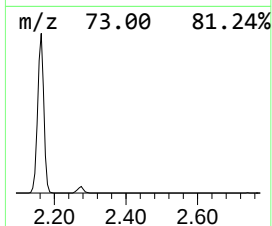
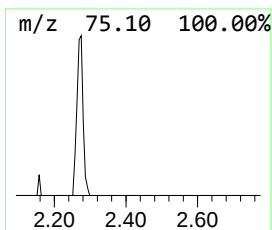
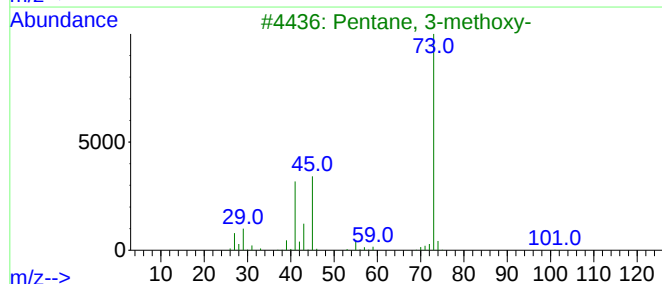
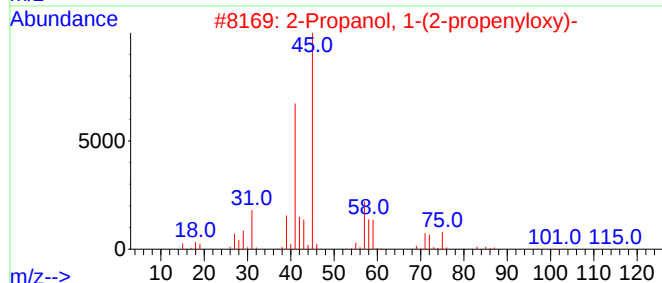
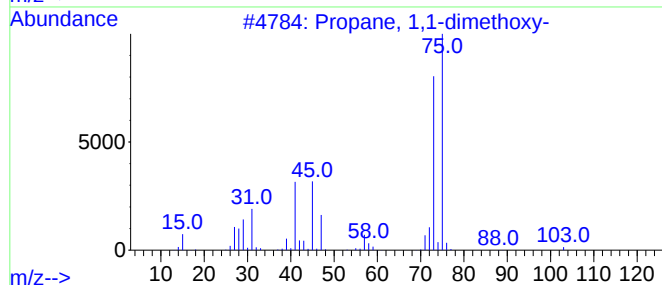
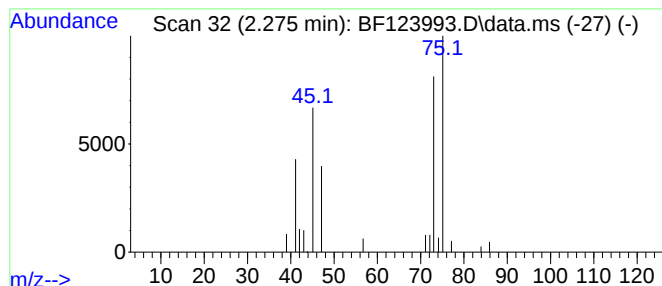
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	3.04 ng	41522	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2			2-Propanol, 1-(2-propenyloxy)-	116	C6H12O2	021460-36-6	9
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	7
5			1-Propene-1-thiol	74	C3H6S	000925-89-3	5



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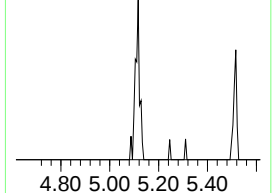
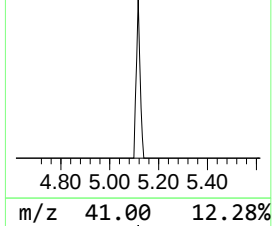
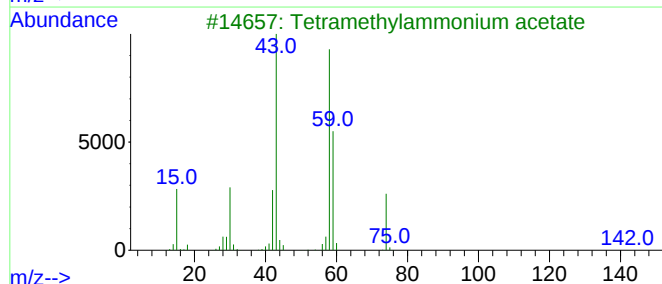
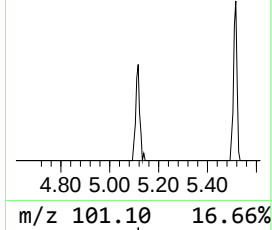
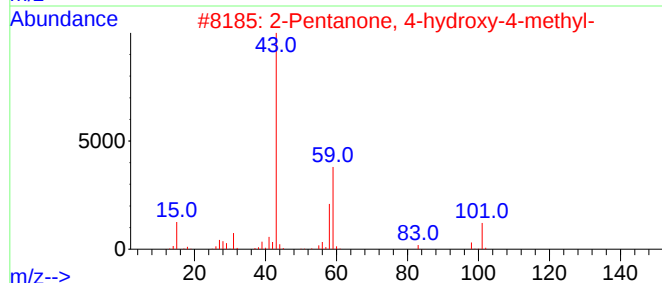
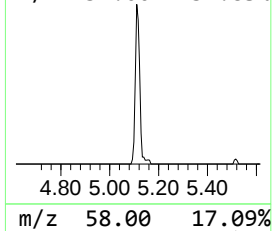
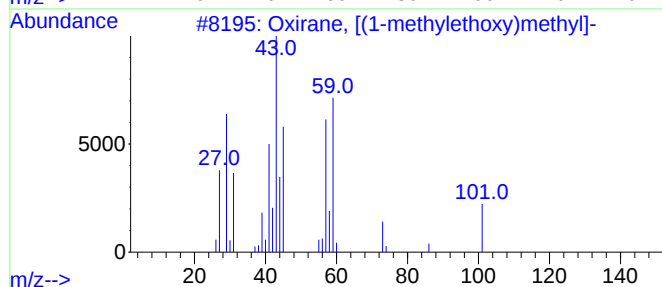
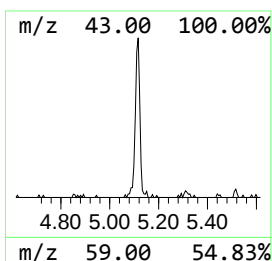
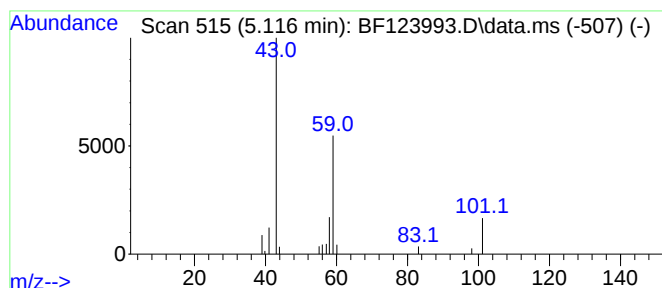
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Oxirane, [(1-methylethoxy)m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	5.83 ng	79594	1,4-Dichlorobenzene-d4	6.904

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	56
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
3		Tetramethylammonium acetate	133	C6H15NO2	010581-12-1	36
4		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	33
5		Diacetamide	101	C4H7NO2	000625-77-4	9



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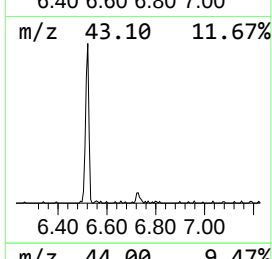
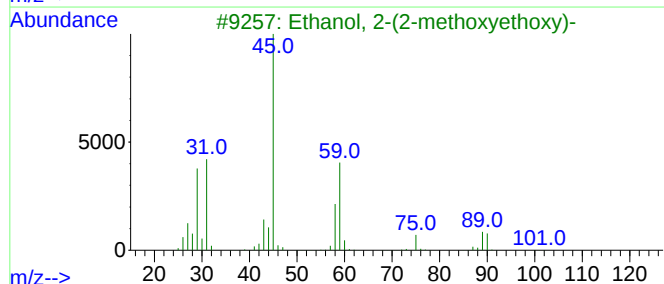
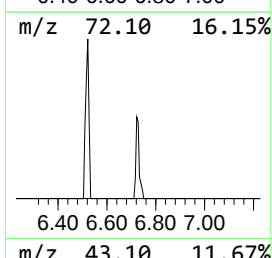
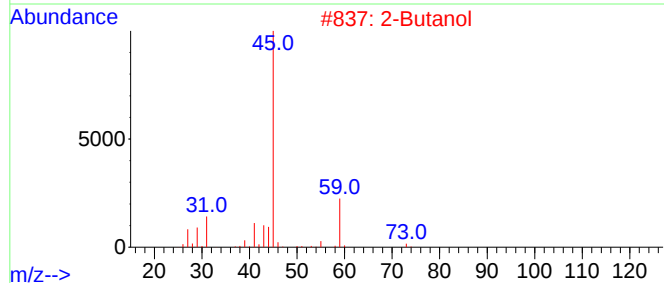
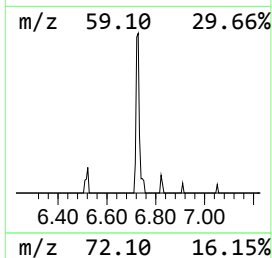
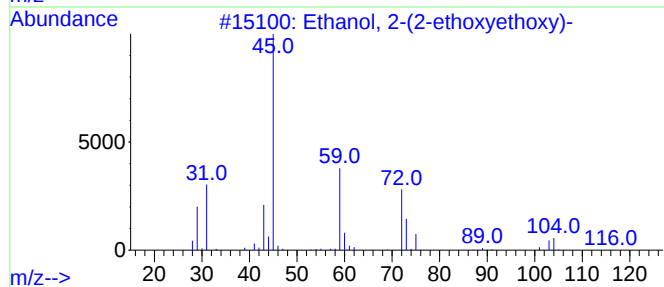
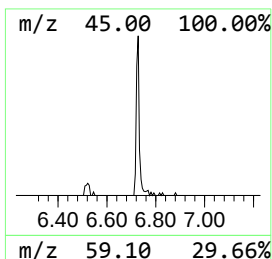
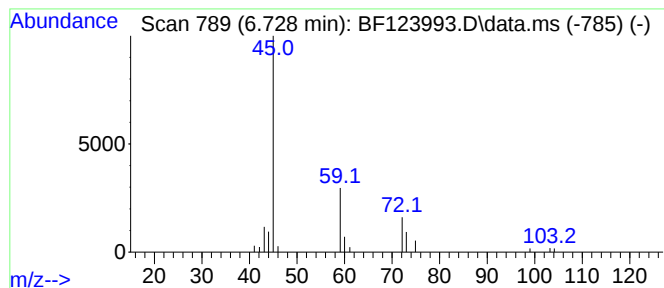
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.728	2.72 ng	37103	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	72
2			2-Butanol	74	C4H10O	000078-92-2	50
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	50
4			2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
5			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	36



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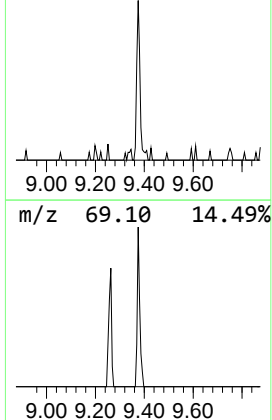
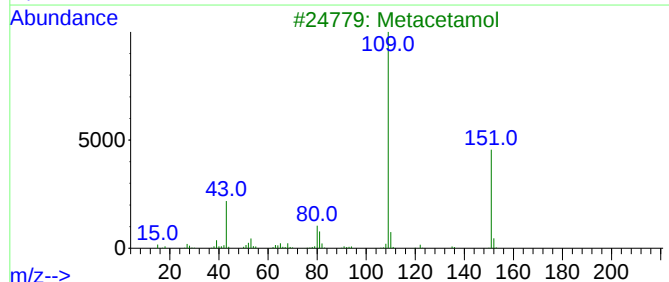
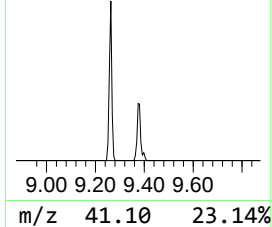
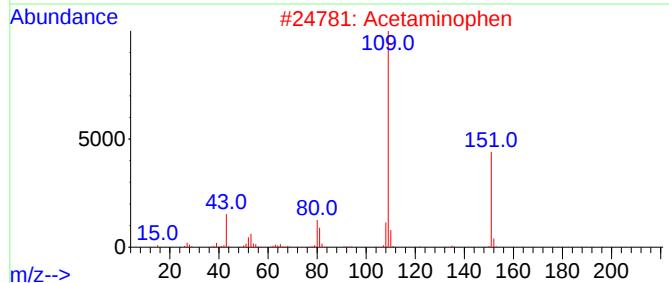
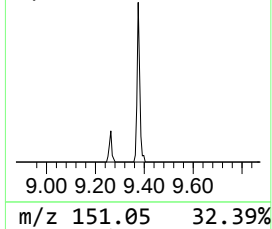
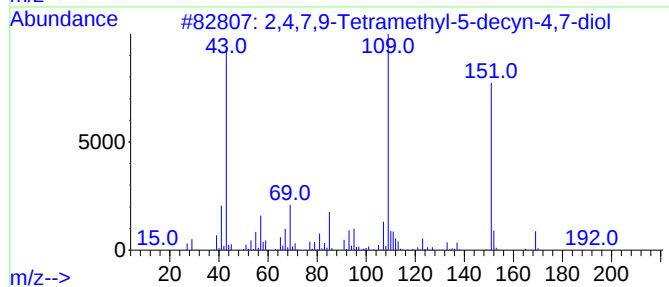
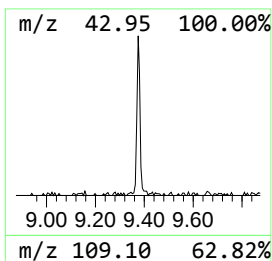
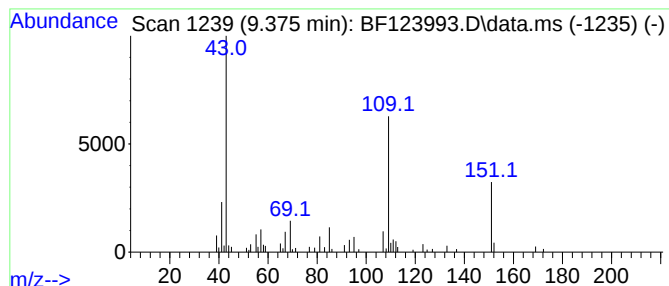
Instrument :
BNA_F
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.375	4.86 ng	99602	Acenaphthene-d10		9.945	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	83
2	Acetaminophen		151	C8H9NO2	000103-90-2	50
3	Metacetamol		151	C8H9NO2	000621-42-1	50
4	m-Isopropoxyaniline		151	C9H13NO	041406-00-2	50
5	Butanamide, N-acetyl-N-(4-hydrox...		221	C12H15NO3	1000107-08-7	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051921\
Data File : BF123993.D
Acq On : 19 May 2021 16:41
Operator : JU/CG
Sample : M2439-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11939

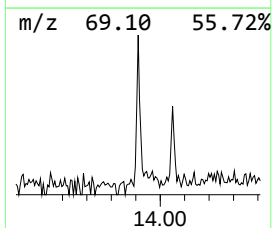
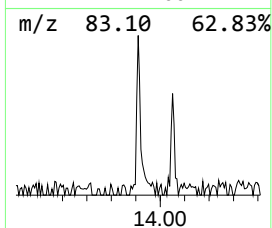
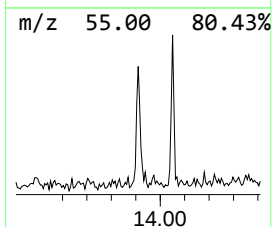
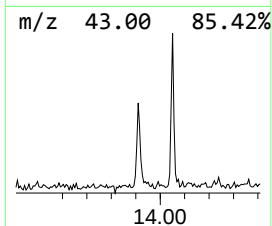
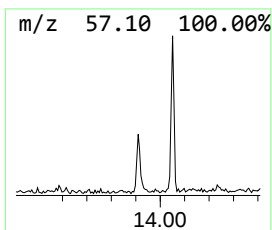
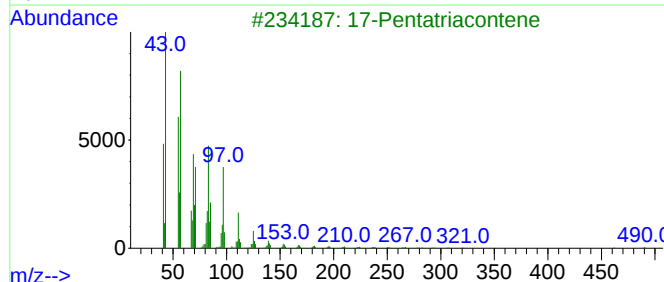
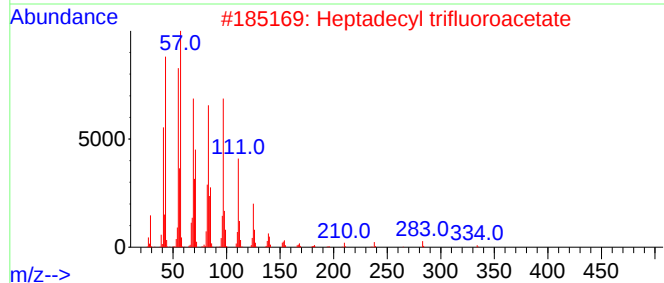
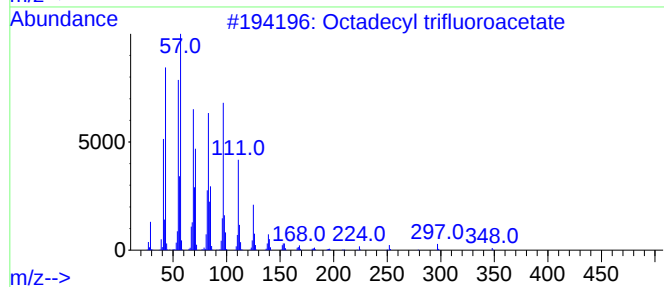
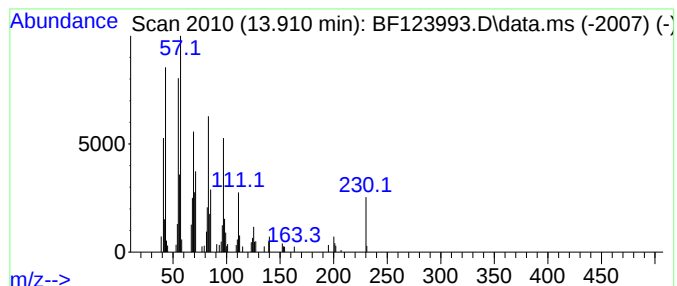
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	10.09 ng	124414	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
3			17-Pentatriacontene	491	C35H70	006971-40-0	87
4			Octacosanol	410	C28H58O	000557-61-9	87
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051921\
Data File : BF123993.D
Acq On : 19 May 2021 16:41
Operator : JU/CG
Sample : M2439-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11939

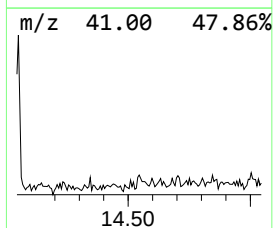
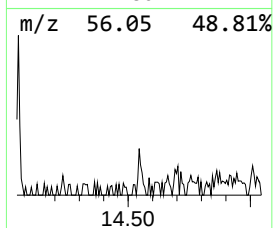
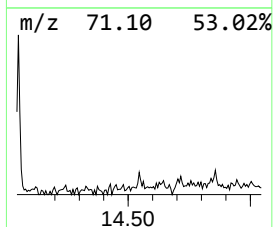
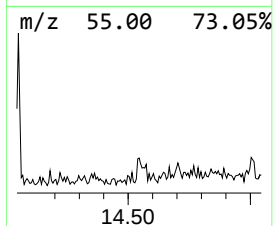
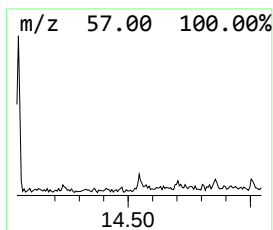
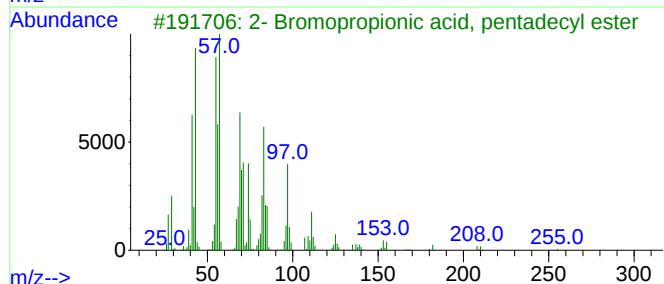
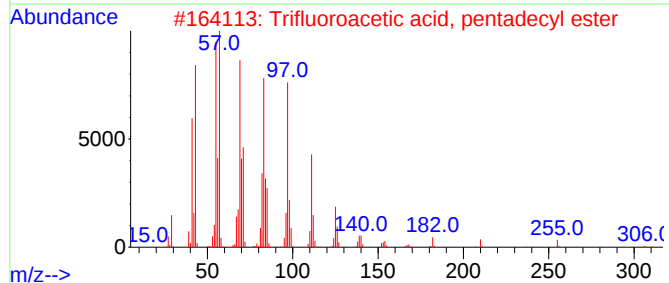
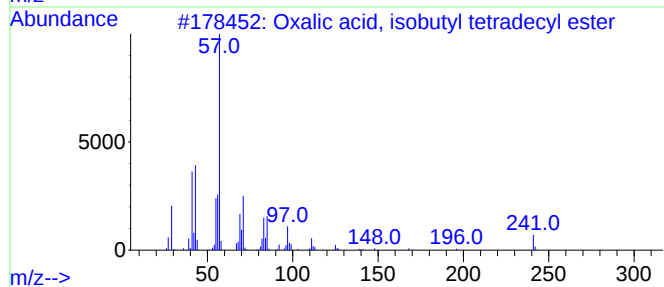
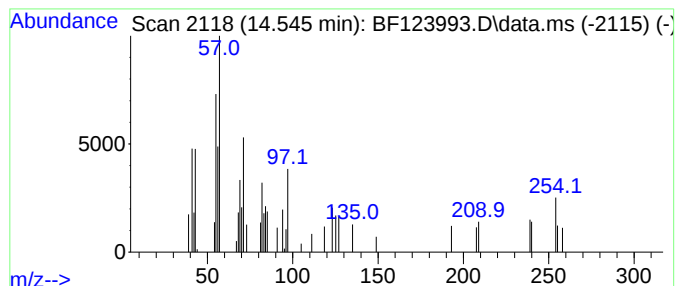
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.545 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	2.13 ng	26283	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	47
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	47
3			2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	38
4			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	38
5			1-Hexadecanethiol	258	C16H34S	002917-26-2	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051921\
Data File : BF123993.D
Acq On : 19 May 2021 16:41
Operator : JU/CG
Sample : M2439-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RO-72-11939

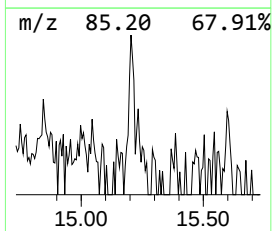
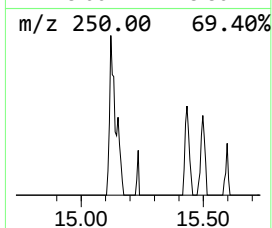
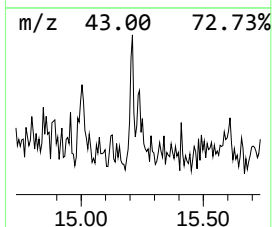
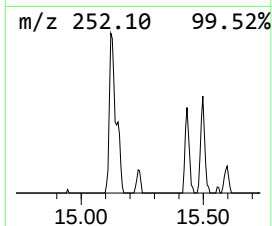
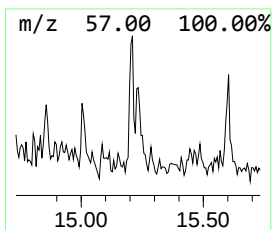
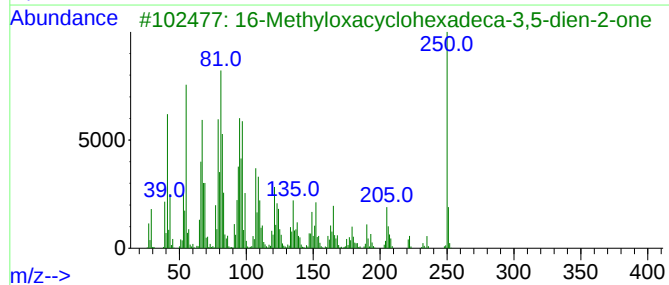
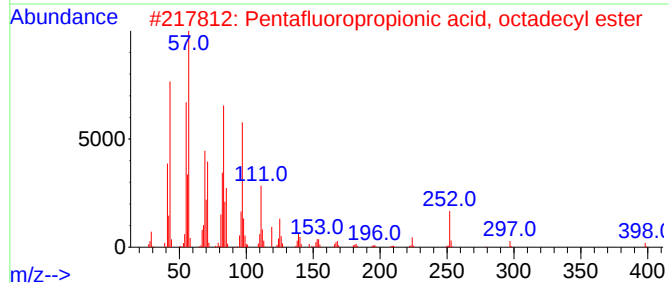
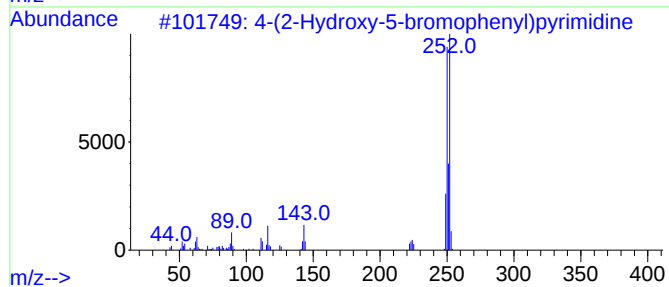
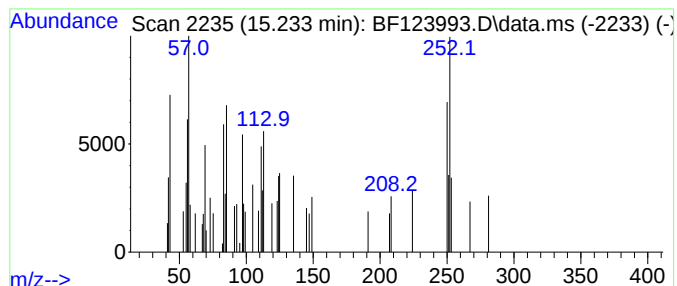
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.233 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	2.39 ng	34692	Perylene-d12	15.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(2-Hydroxy-5-bromophenyl)pyrim...	250	C10H7BrN2O	097630-76-7	27
2			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	25
3			16-Methyloxacyclohexadeca-3,5-di...	250	C16H26O2	087295-26-9	25
4			E-7-Octadecene	252	C18H36	1000130-92-0	25
5			Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051921\
Data File : BF123993.D
Acq On : 19 May 2021 16:41
Operator : JU/CG
Sample : M2439-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11939

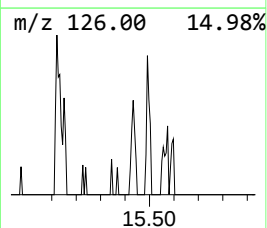
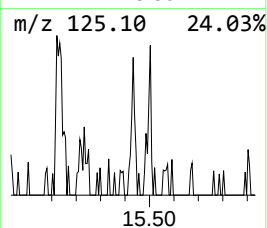
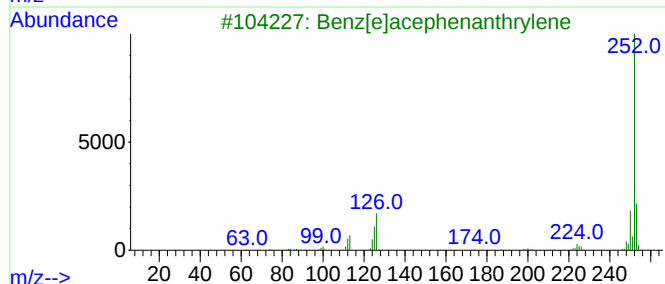
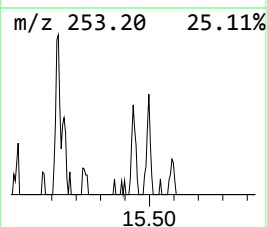
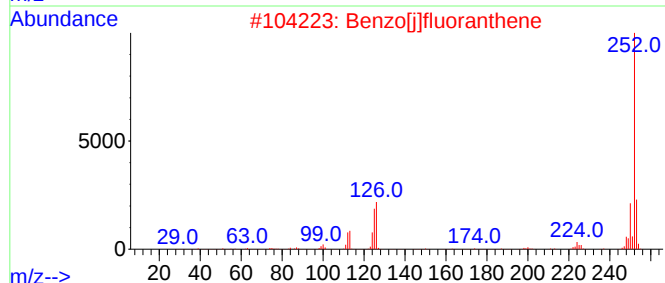
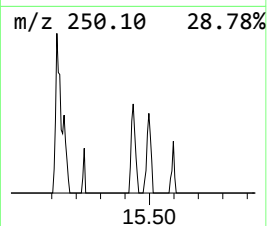
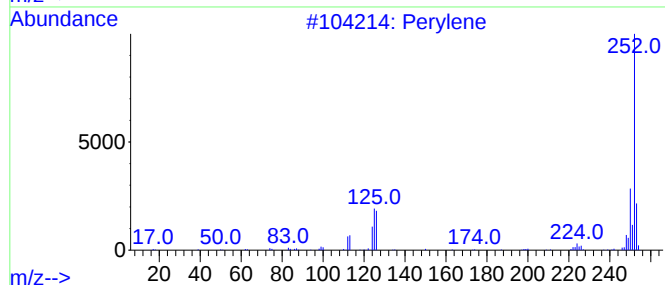
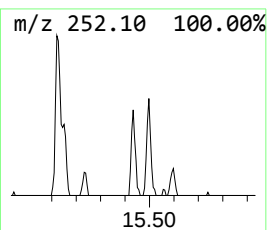
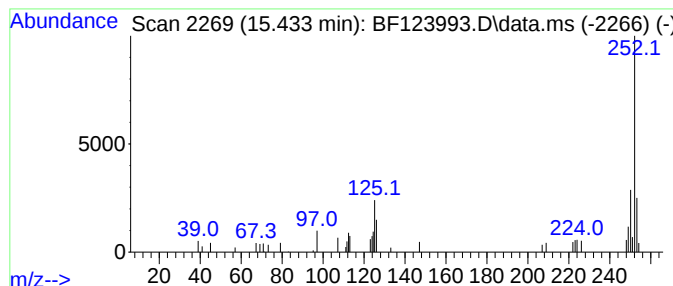
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.433	2.26 ng	32739	Perylene-d12	15.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	72
2			Benzo[j]fluoranthene	252	C20H12	000205-82-3	72
3			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	68
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	64
5			Benzo[e]pyrene	252	C20H12	000192-97-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051921\
Data File : BF123993.D
Acq On : 19 May 2021 16:41
Operator : JU/CG
Sample : M2439-01
Misc :
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ClientSampleId :
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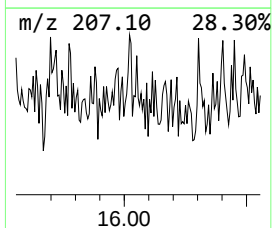
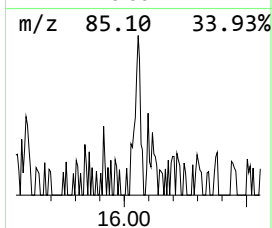
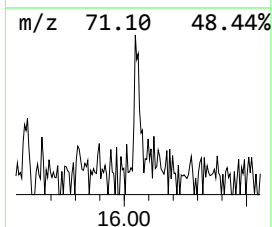
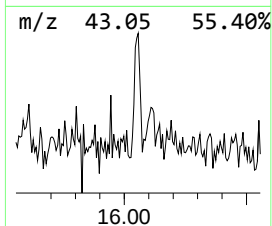
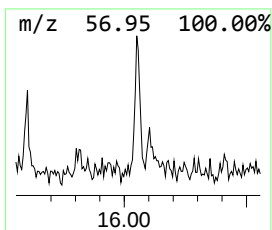
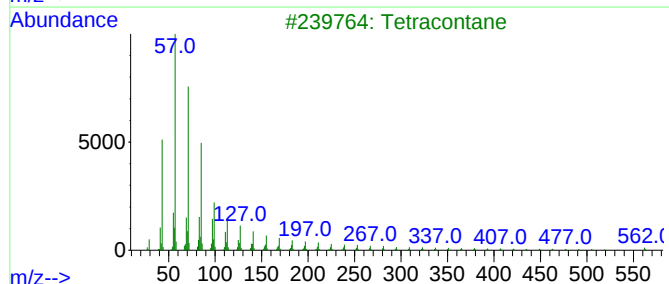
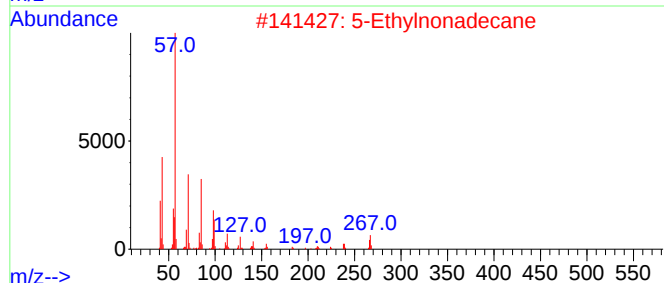
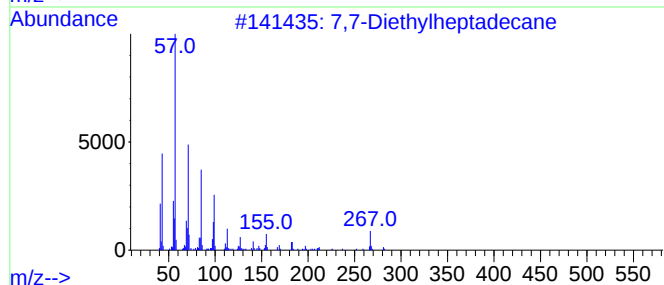
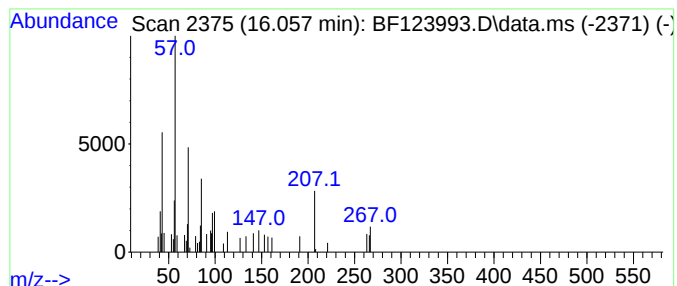
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 7,7-Diethylheptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.057	2.15 ng	31134	Perylene-d12	15.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7,7-Diethylheptadecane	296	C21H44	1000360-41-5	53
2			5-Ethylnonadecane	296	C21H44	1000360-43-1	53
3			Tetracontane	563	C40H82	004181-95-7	50
4			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	47
5			Octacosane	394	C28H58	000630-02-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051921\
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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
Butane, 2-metho...	2.163	40.5	ng	553750	1	6.904	273116	20.0
Propane, 1,1-di...	2.275	3.0	ng	41522	1	6.904	273116	20.0
Oxirane, [(1-me...	5.116	5.8	ng	79594	1	6.904	273116	20.0
Ethanol, 2-(2-e...	6.728	2.7	ng	37103	1	6.904	273116	20.0
2,4,7,9-Tetrame...	9.375	4.9	ng	99602	3	9.945	410257	20.0
Octadecyl trifl...	13.910	10.1	ng	124414	5	14.068	246629	20.0
unknown14.545	14.545	2.1	ng	26283	5	14.068	246629	20.0
unknown15.233	15.233	2.4	ng	34692	6	15.562	290275	20.0
Perylene	15.433	2.3	ng	32739	6	15.562	290275	20.0
7,7-Diethylhept...	16.057	2.1	ng	31134	6	15.562	290275	20.0