

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091724\
 Data File : BF139407.D
 Acq On : 17 Sep 2024 17:36
 Operator : RC/JU
 Sample : P4002-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2

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-BF091324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139407.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	9	18	25	rVB	862064	1341678	75.12%	9.301%
2	5.104	502	512	524	rVB	78308	123810	6.93%	0.858%
3	5.498	573	579	585	rBV	1274679	1758082	98.43%	12.188%
4	6.504	744	750	756	rBV	1247800	1786040	100.00%	12.381%
5	6.875	808	813	818	rVB	297876	372021	20.83%	2.579%
6	7.439	902	909	914	rBV	891674	1165159	65.24%	8.077%
7	7.692	948	952	961	rVB	33837	40867	2.29%	0.283%
8	8.157	1026	1031	1039	rBV	354825	448911	25.13%	3.112%
9	9.233	1208	1214	1219	rBV	1446616	1761812	98.64%	12.213%
10	9.398	1238	1242	1250	rVB	12664	18594	1.04%	0.129%
11	9.910	1324	1329	1338	rBV2	327105	429170	24.03%	2.975%
12	10.251	1368	1387	1389	rBV2	7090	32736	1.83%	0.227%
13	10.622	1446	1450	1456	rVB	83834	101501	5.68%	0.704%
14	10.698	1458	1463	1468	rBV	686762	861941	48.26%	5.975%
15	11.398	1577	1582	1590	rBV2	254033	436922	24.46%	3.029%
16	11.469	1591	1594	1598	rVB	21220	25455	1.43%	0.176%
17	11.551	1604	1608	1614	rBV2	17809	30008	1.68%	0.208%
18	11.922	1664	1671	1676	rBV2	122180	187175	10.48%	1.298%
19	12.010	1683	1686	1693	rVB	27705	52499	2.94%	0.364%
20	12.604	1783	1787	1792	rBV	157856	197855	11.08%	1.372%
21	12.704	1800	1804	1808	rBV	23994	34021	1.90%	0.236%
22	12.833	1820	1826	1832	rBV	146706	218955	12.26%	1.518%
23	12.980	1845	1851	1857	rVB	976686	1245107	69.71%	8.632%
24	13.057	1859	1864	1868	rVV3	15757	27087	1.52%	0.188%
25	13.157	1875	1881	1885	rBV	37130	64682	3.62%	0.448%
26	13.227	1890	1893	1896	rVV	23493	26542	1.49%	0.184%
27	13.263	1896	1899	1904	rVB2	19274	23534	1.32%	0.163%
28	13.357	1912	1915	1918	rBV	22778	28351	1.59%	0.197%
29	13.386	1918	1920	1924	rVB	19251	22810	1.28%	0.158%
30	13.780	1982	1987	1989	rBV3	16464	29052	1.63%	0.201%
31	13.868	1998	2002	2011	rVB2	103198	161527	9.04%	1.120%
32	14.027	2023	2029	2040	rVB2	272772	532435	29.81%	3.691%
33	14.504	2105	2110	2124	rVB2	80701	173933	9.74%	1.206%
34	15.068	2201	2206	2215	rBV	71783	161302	9.03%	1.118%
35	15.174	2222	2224	2230	rVB	14585	18253	1.02%	0.127%
36	15.374	2253	2258	2264	rBV	53966	85127	4.77%	0.590%

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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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.433	2264	2268	2273	rVB	48393	74028	4.14%	0.513%
38	15.498	2274	2279	2291	rVB	120480	219816	12.31%	1.524%
39	16.962	2522	2528	2536	rVB2	25370	55273	3.09%	0.383%
40	17.404	2598	2603	2617	rVB2	20105	51066	2.86%	0.354%

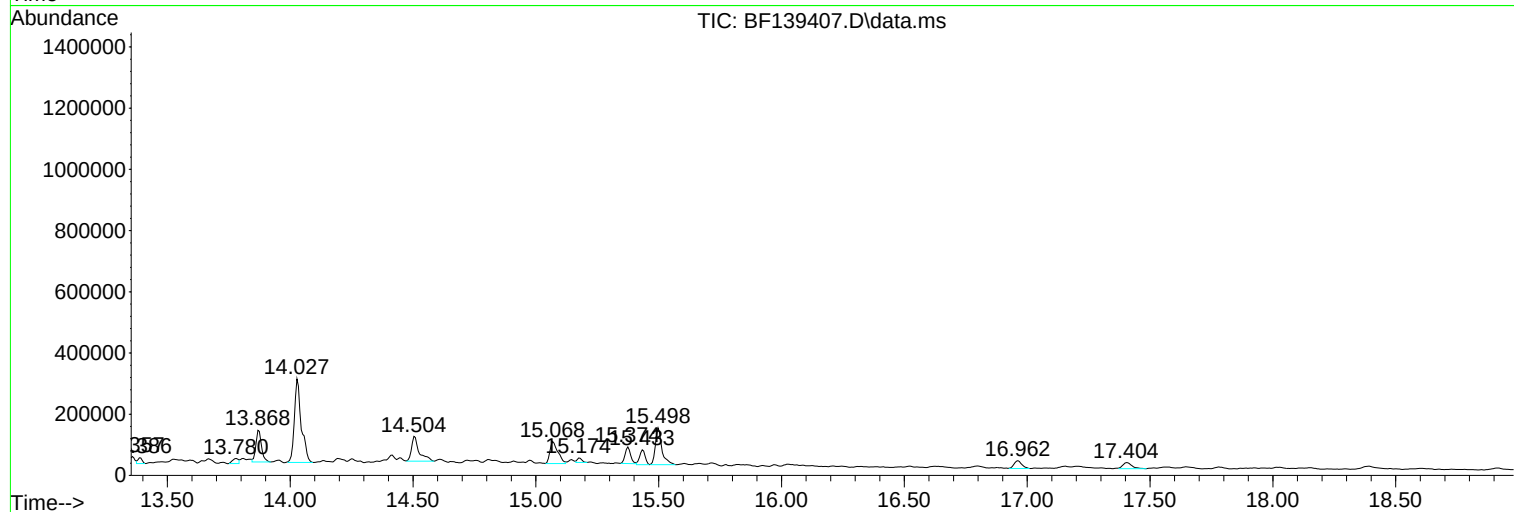
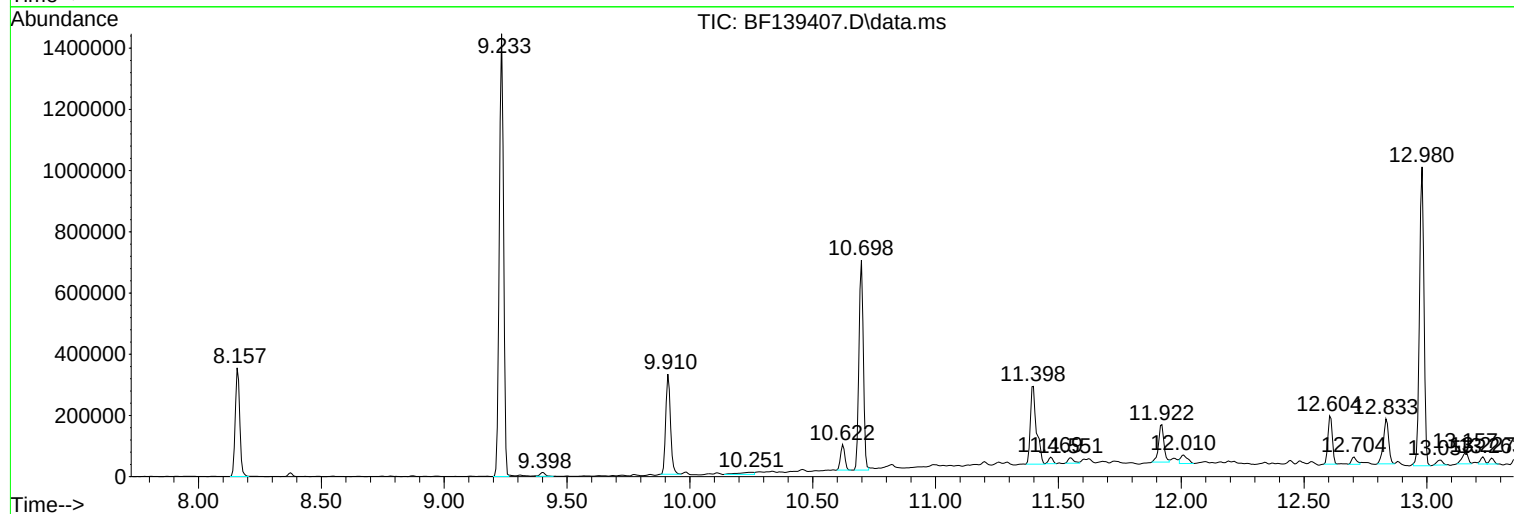
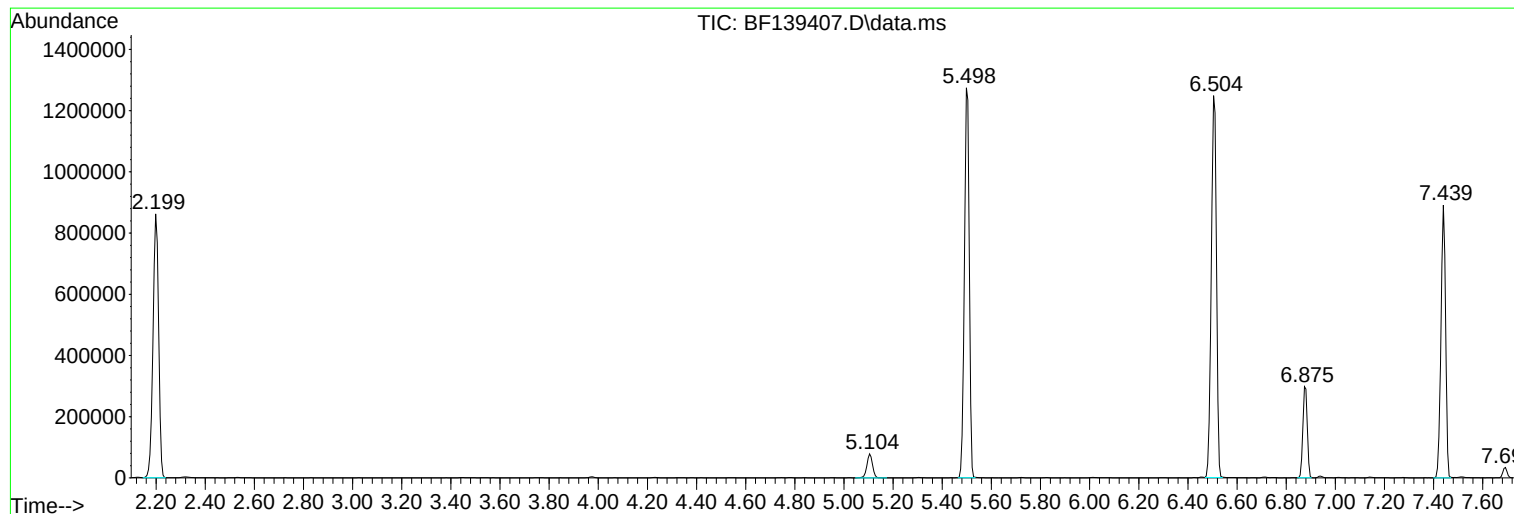
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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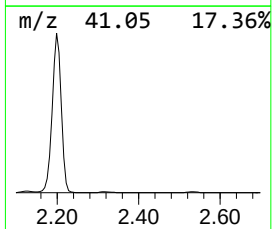
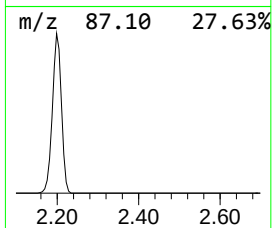
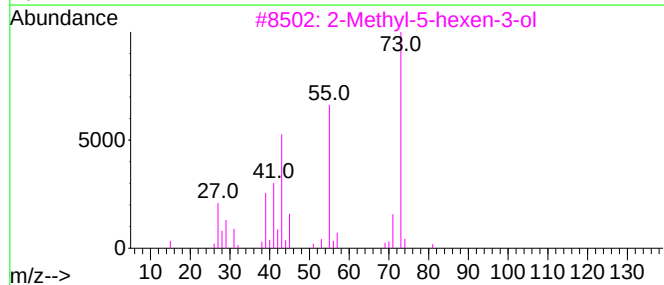
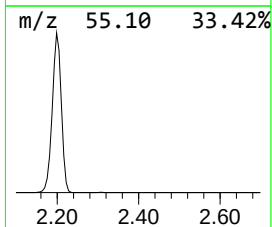
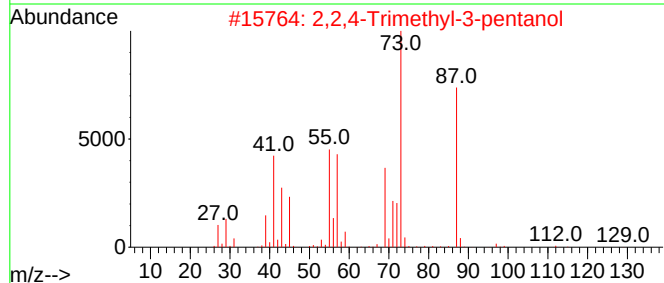
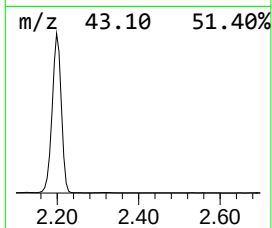
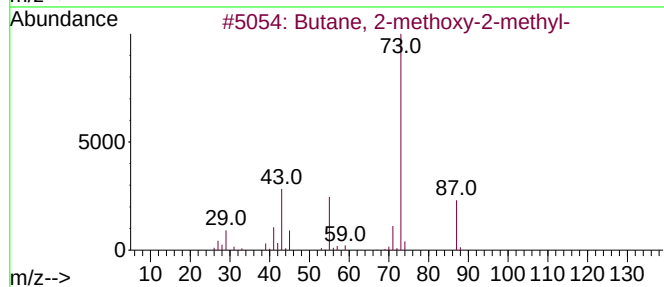
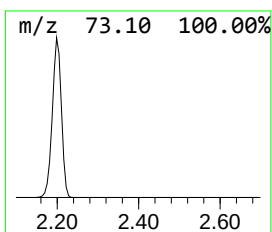
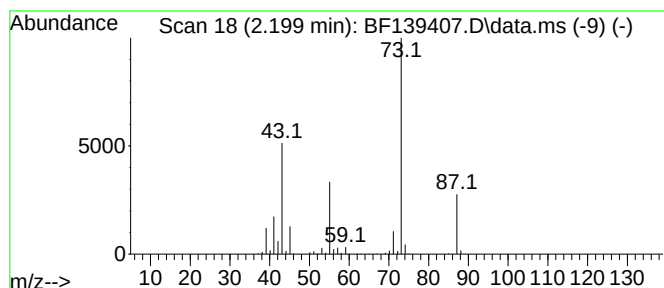
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
2.199	72.13 ng	1341680	1,4-Dichlorobenzene-d4	6.881

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	40
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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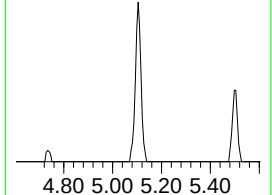
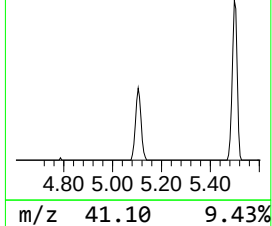
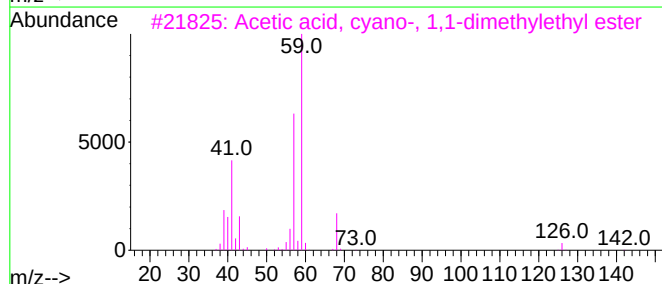
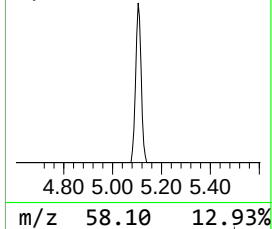
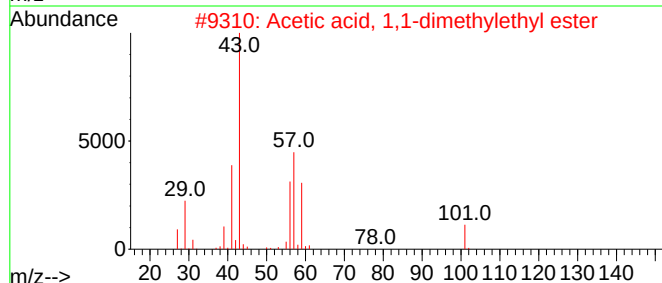
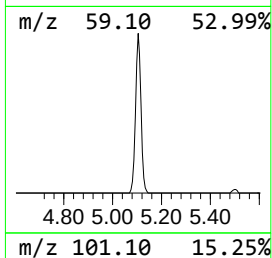
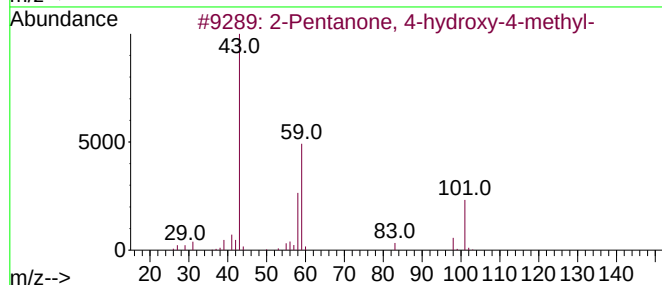
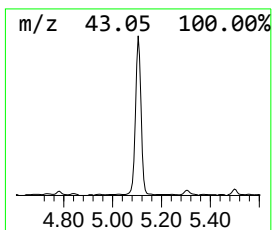
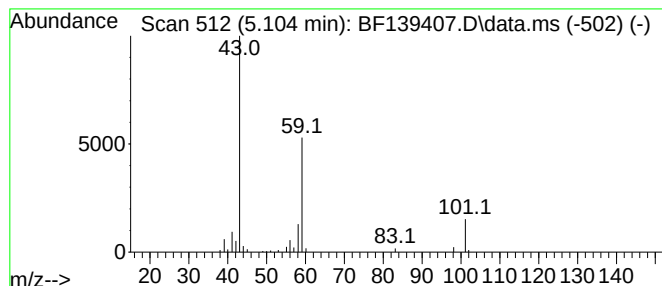
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	6.66 ng	123810	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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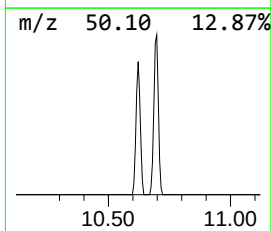
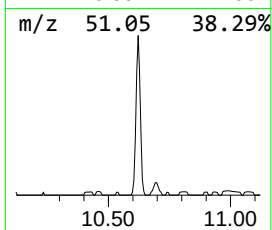
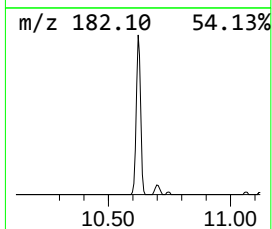
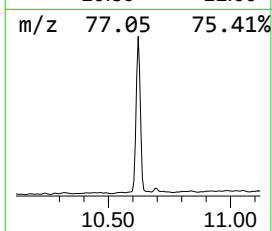
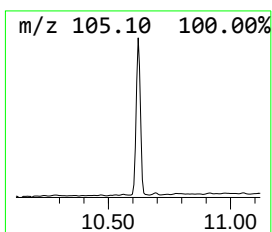
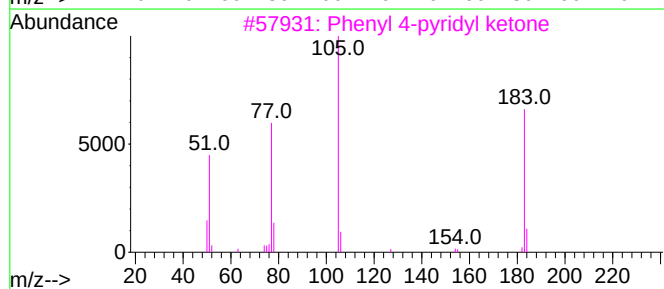
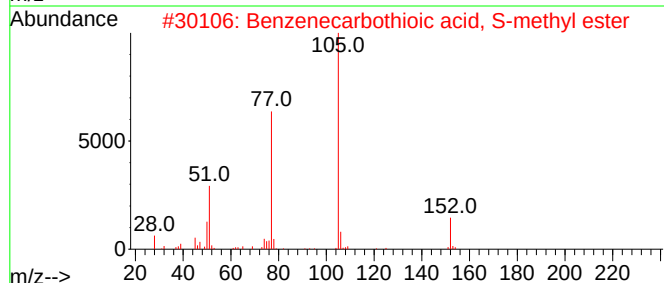
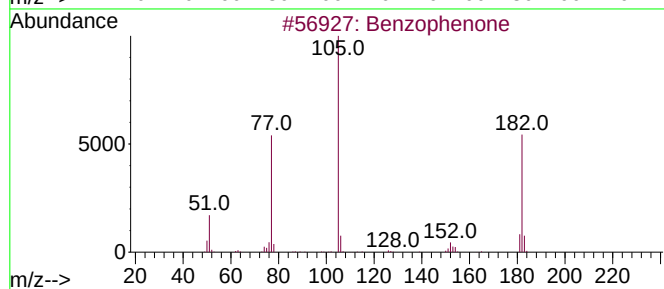
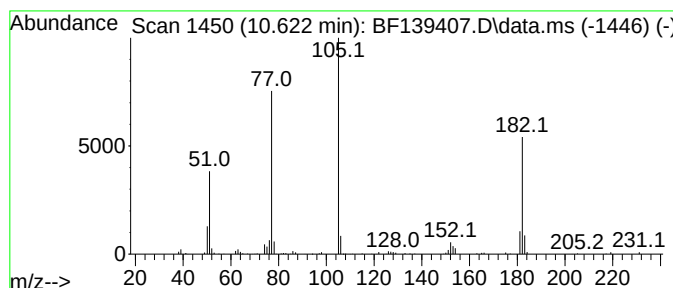
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.622	4.73 ng	101501	Acenaphthene-d10	9.910	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	62
3	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	62
4	5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	53
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	53



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Instrument :
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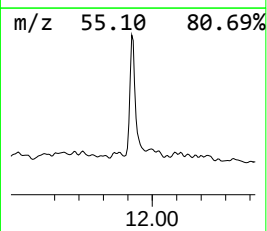
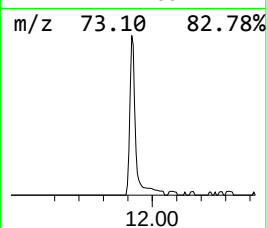
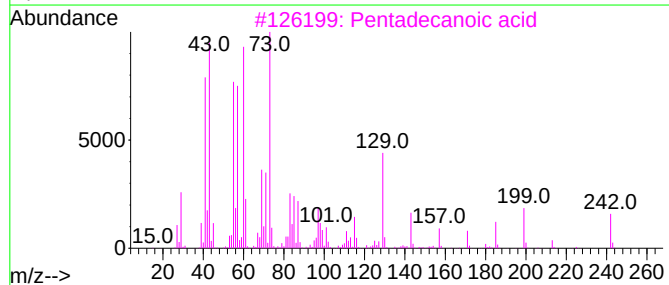
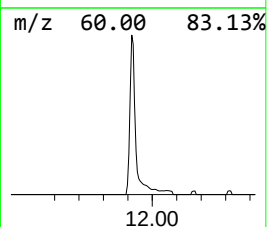
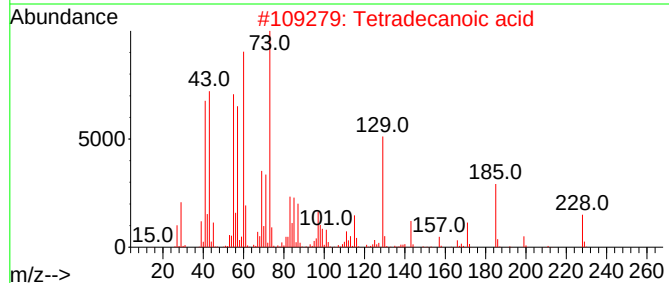
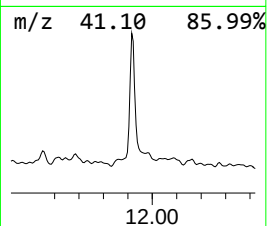
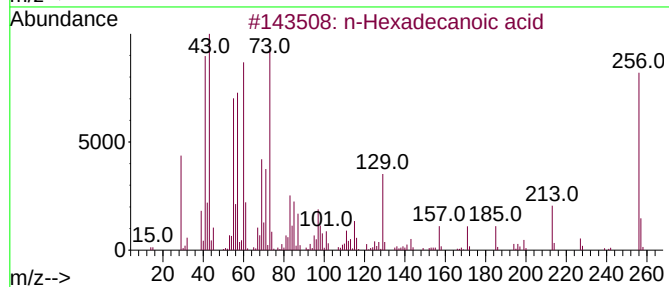
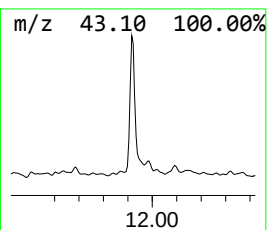
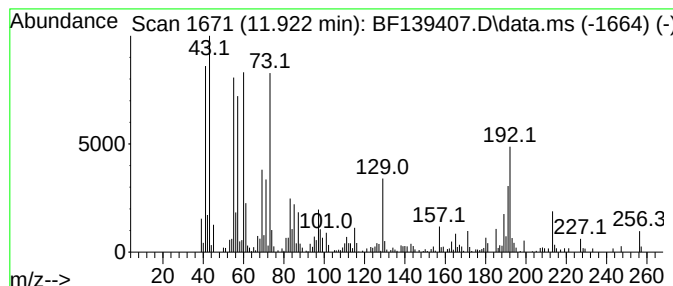
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	8.57 ng	187175	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4			Tridecanoic acid	214	C13H26O2	000638-53-9	58
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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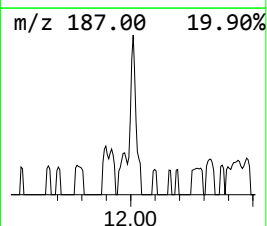
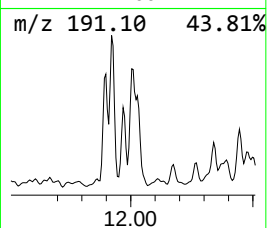
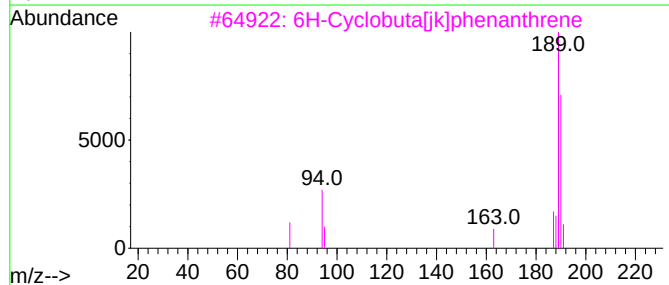
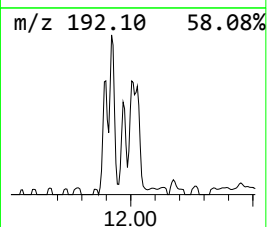
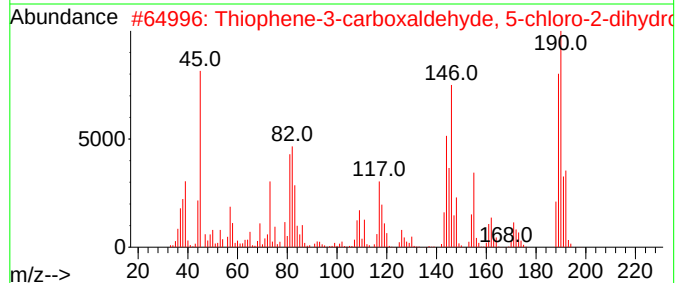
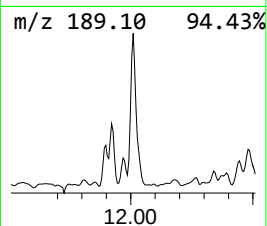
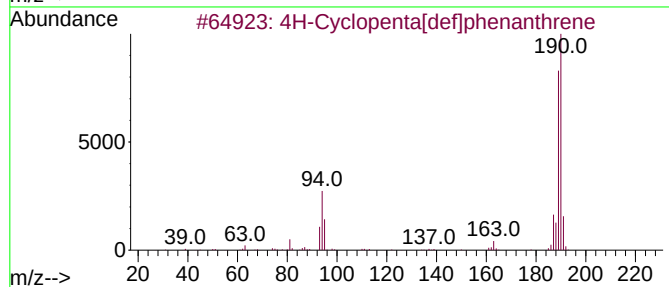
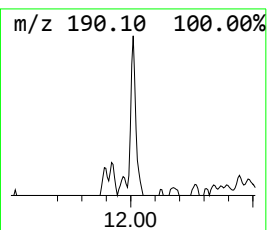
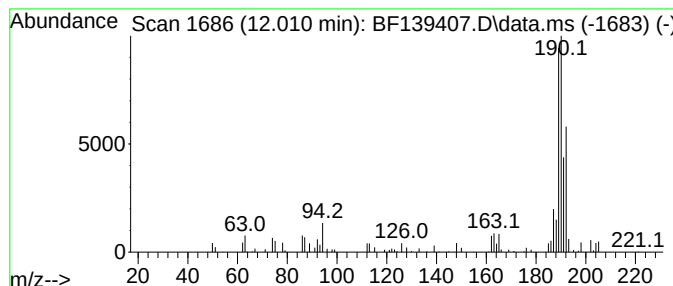
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	2.40 ng	52499	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
3			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
4			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	40
5			2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091724\
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Acq On : 17 Sep 2024 17:36
Operator : RC/JU
Sample : P4002-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-2

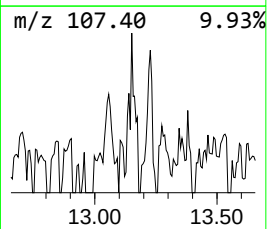
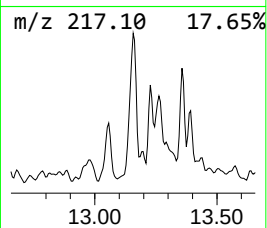
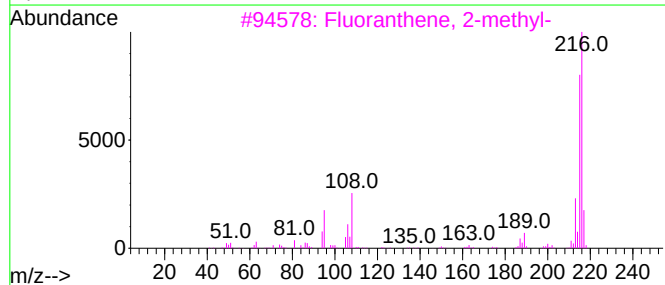
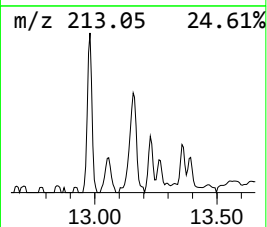
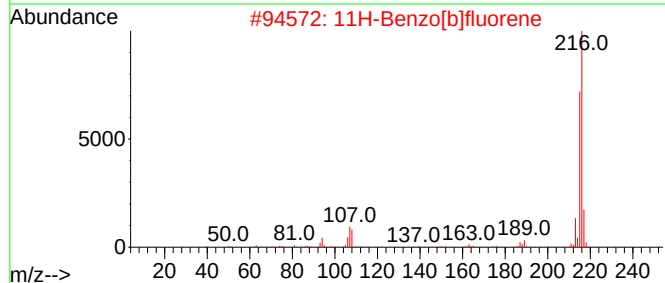
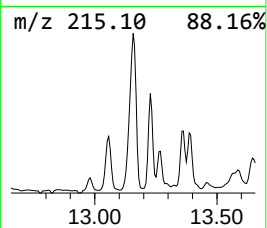
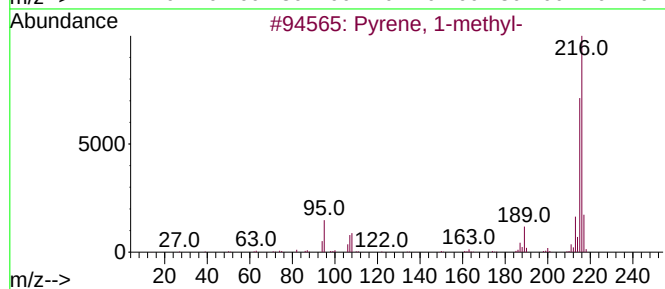
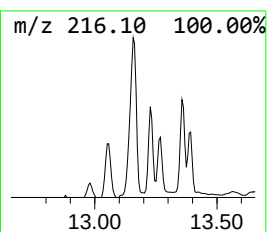
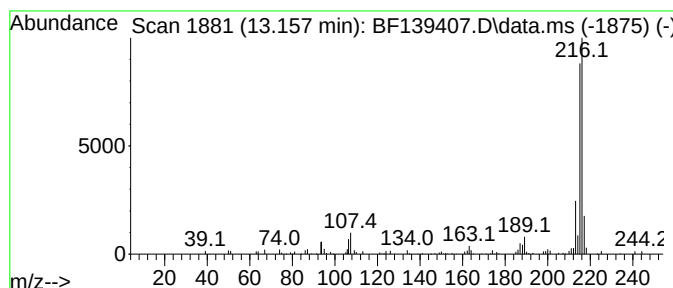
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	2.43 ng	64682	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
4			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091724\
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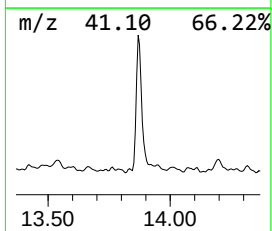
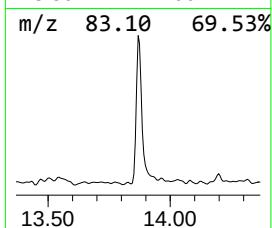
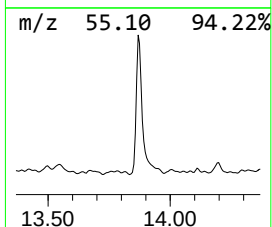
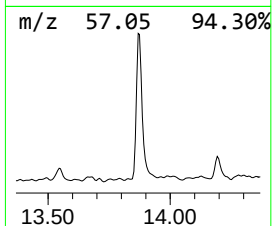
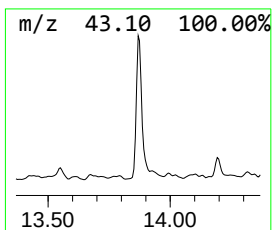
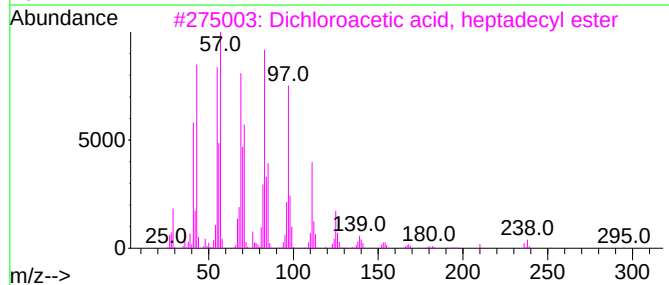
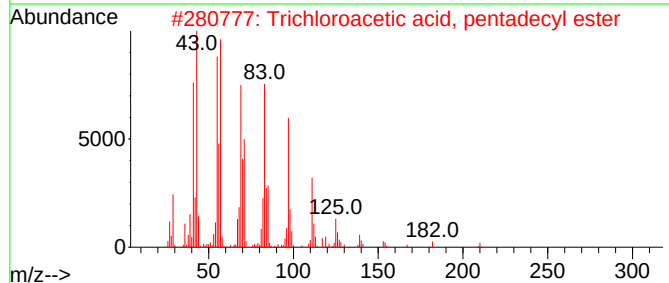
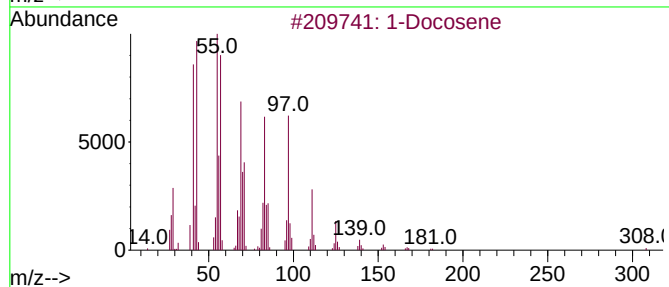
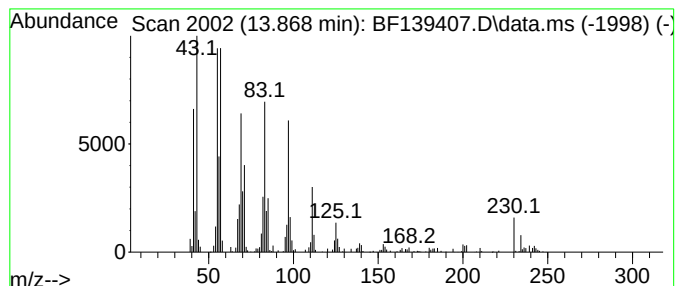
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	6.07 ng	161527	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	93
2	Trichloroacetic acid, pentadecyl...			372	C17H31Cl3O2	074339-53-0	93
3	Dichloroacetic acid, heptadecyl ...			366	C19H36Cl2O2	1000282-98-2	93
4	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	93
5	Heptadecyl trifluoroacetate			352	C19H35F3O2	1010351-87-0	93



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Sample : P4002-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

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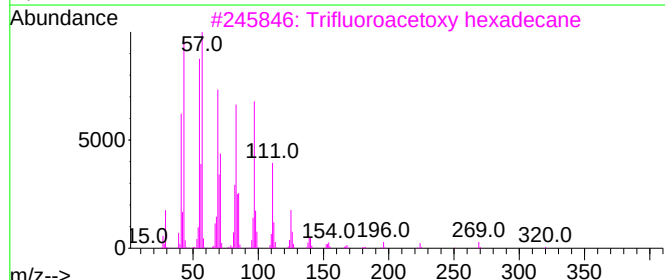
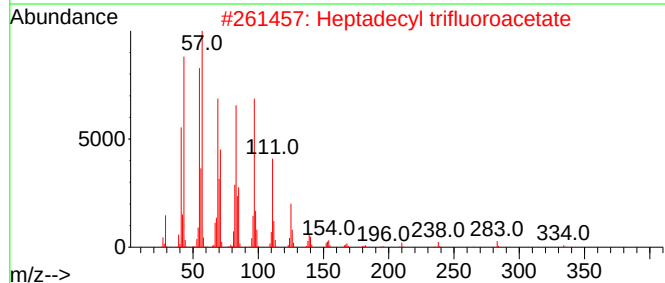
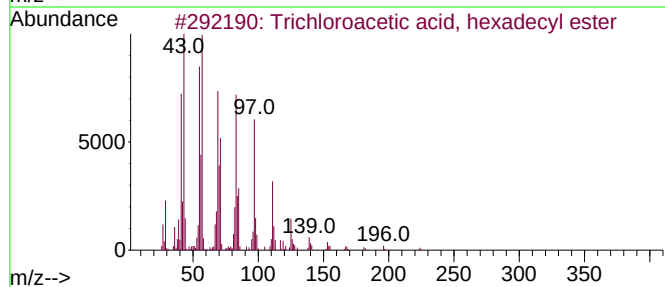
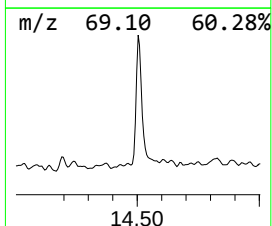
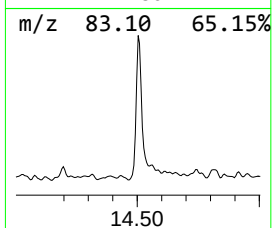
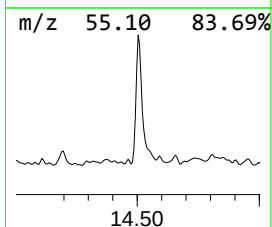
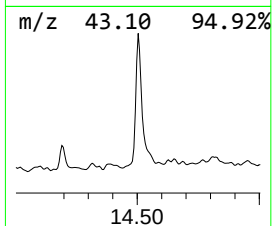
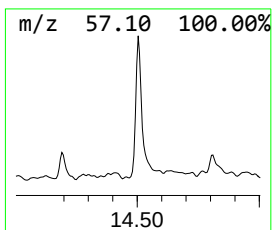
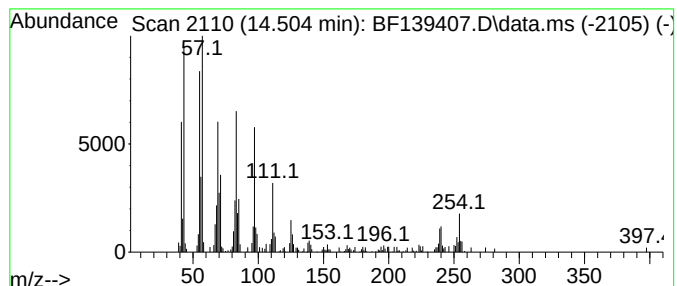
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	6.53 ng	173933	Chrysene-d12	14.033

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	93
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4			1-Heneicosanol	312	C21H44O	015594-90-8	92
5			E-15-Heptadecenal	252	C17H32O	1000130-97-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091724\
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Sample : P4002-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

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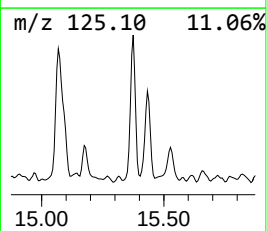
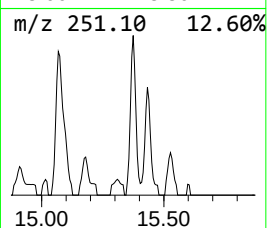
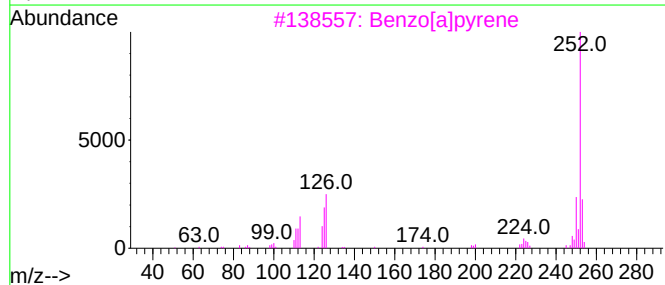
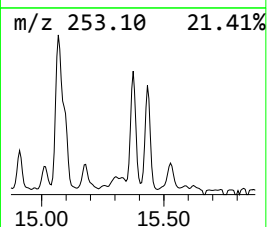
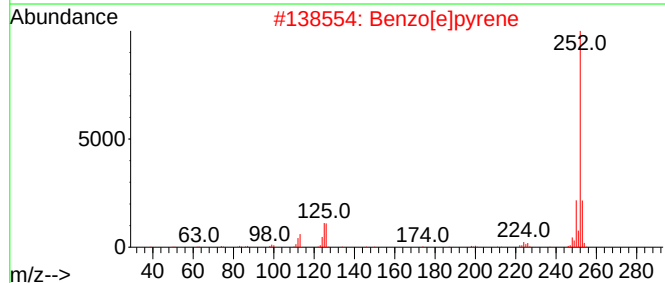
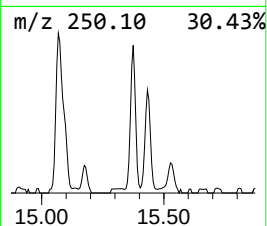
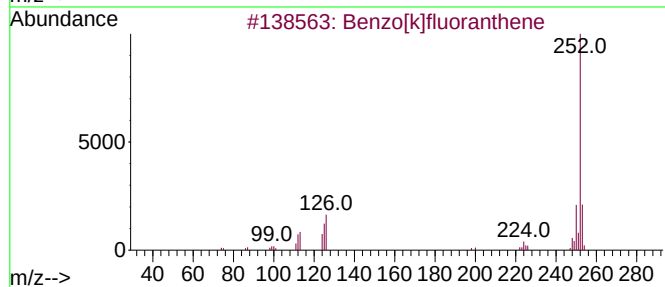
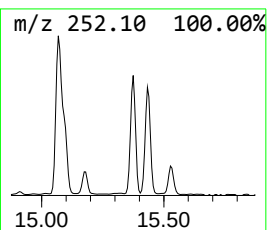
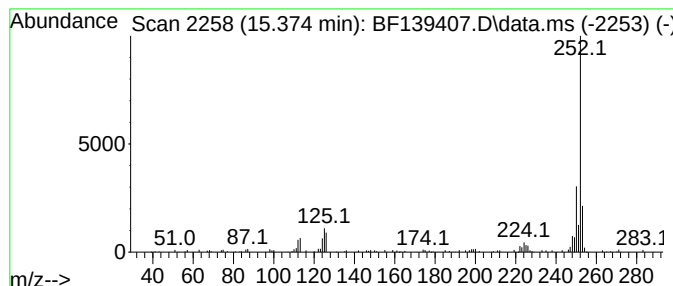
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	7.75 ng	85127	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
2			Benzo[e]pyrene	252	C20H12	000192-97-2	93
3			Benzo[a]pyrene	252	C20H12	000050-32-8	90
4			Perylene	252	C20H12	000198-55-0	90
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091724\
Data File : BF139407.D
Acq On : 17 Sep 2024 17:36
Operator : RC/JU
Sample : P4002-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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
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2-Pentanone, 4-...	5.104	6.7	ng	123810	1	6.881	372021	20.0
Benzophenone	10.622	4.7	ng	101501	3	9.910	429170	20.0
n-Hexadecanoic ...	11.922	8.6	ng	187175	4	11.398	436922	20.0
4H-Cyclopenta[d...]	12.010	2.4	ng	52499	4	11.398	436922	20.0
Pyrene, 1-methyl-	13.157	2.4	ng	64682	5	14.033	532435	20.0
1-Docosene	13.868	6.1	ng	161527	5	14.033	532435	20.0
Trichloroacetic...	14.504	6.5	ng	173933	5	14.033	532435	20.0
Benzo[e]pyrene	15.374	7.8	ng	85127	6	15.498	219816	20.0