

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
 Data File : BF139439.D
 Acq On : 18 Sep 2024 21:41
 Operator : RC/JU
 Sample : P4087-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-614-COMP-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-BF091324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139439.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	13	20	rVB	490784	755987	61.28%	7.111%
2	5.093	500	510	522	rBB	82358	122274	9.91%	1.150%
3	5.493	572	578	583	rBV	846176	1091765	88.50%	10.270%
4	6.504	744	750	755	rBV	906576	1175773	95.31%	11.060%
5	6.875	809	813	818	rBV	304215	381083	30.89%	3.585%
6	7.440	903	909	914	rBV	599533	757309	61.39%	7.124%
7	7.692	947	952	958	rVB	15297	18426	1.49%	0.173%
8	8.157	1026	1031	1039	rBV	365623	453869	36.79%	4.269%
9	9.234	1208	1214	1219	rBV	1009661	1233584	100.00%	11.604%
10	9.910	1324	1329	1334	rBV	338870	413762	33.54%	3.892%
11	10.004	1339	1345	1359	rVB	214303	319523	25.90%	3.006%
12	10.622	1445	1450	1458	rBV	41347	49921	4.05%	0.470%
13	10.698	1458	1463	1473	rBV	446514	564502	45.76%	5.310%
14	11.398	1576	1582	1590	rBV	281801	406343	32.94%	3.822%
15	11.892	1662	1666	1667	rBV	24318	23816	1.93%	0.224%
16	11.916	1667	1670	1682	rVV3	74030	124440	10.09%	1.171%
17	12.004	1682	1685	1694	rVB2	14706	29568	2.40%	0.278%
18	12.127	1702	1706	1711	rVB3	23434	34081	2.76%	0.321%
19	12.216	1713	1721	1727	rVB5	11918	23988	1.94%	0.226%
20	12.422	1753	1756	1759	rBV2	16017	20475	1.66%	0.193%
21	12.604	1778	1787	1795	rBV	106973	156925	12.72%	1.476%
22	12.698	1799	1803	1807	rVB	109285	134714	10.92%	1.267%
23	12.804	1816	1821	1823	rBV	106549	149986	12.16%	1.411%
24	12.833	1823	1826	1833	rVB	101762	149104	12.09%	1.403%
25	12.980	1845	1851	1858	rVB	716963	942632	76.41%	8.867%
26	13.051	1858	1863	1868	rBV3	10693	19721	1.60%	0.186%
27	13.157	1875	1881	1885	rVB2	10949	22547	1.83%	0.212%
28	13.263	1896	1899	1903	rVB2	11656	15651	1.27%	0.147%
29	13.669	1965	1968	1972	rVB	14401	18573	1.51%	0.175%
30	13.780	1983	1987	1990	rBV2	11324	16993	1.38%	0.160%
31	13.874	1999	2003	2014	rVB	60086	100755	8.17%	0.948%
32	14.027	2022	2029	2040	rBV2	260510	483542	39.20%	4.548%
33	15.074	2202	2207	2215	rBV	43803	101322	8.21%	0.953%
34	15.374	2255	2258	2264	rVB	28024	44088	3.57%	0.415%
35	15.433	2265	2268	2274	rVB	31445	45360	3.68%	0.427%
36	15.498	2274	2279	2290	rBV	137773	228725	18.54%	2.151%

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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

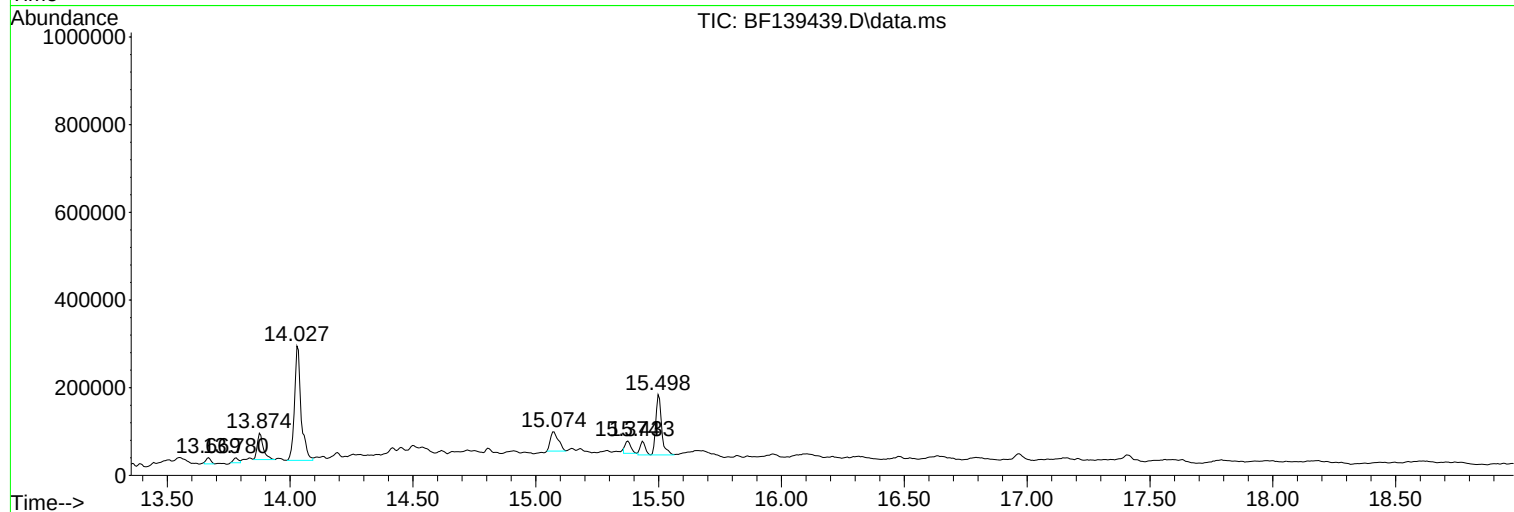
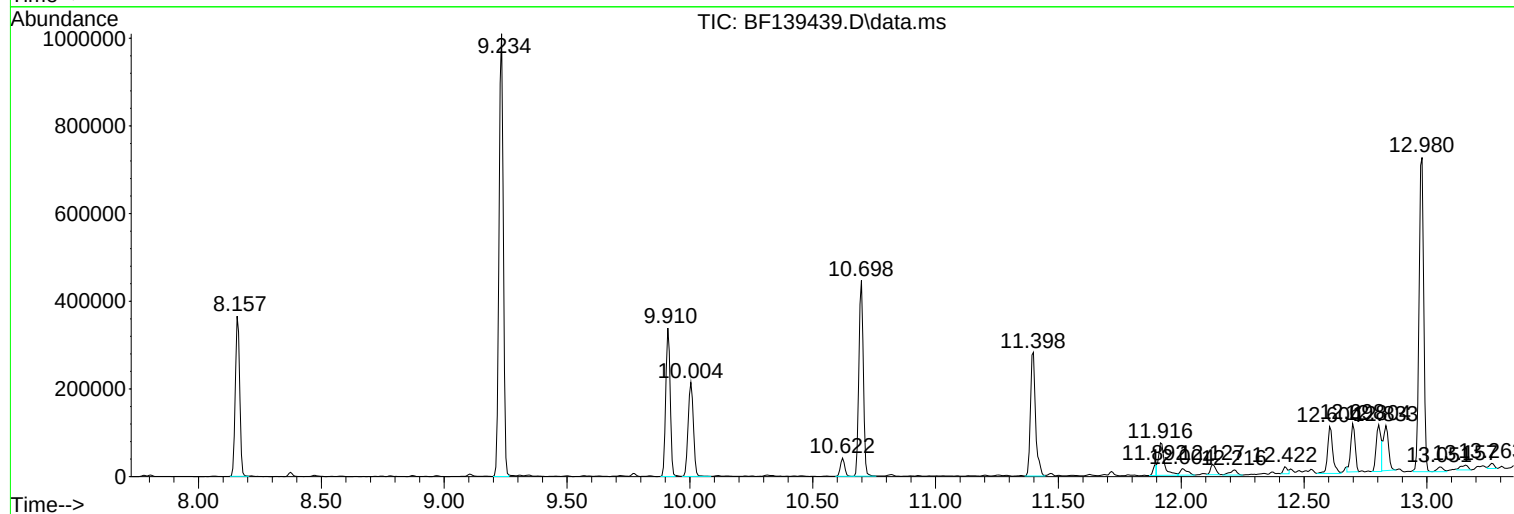
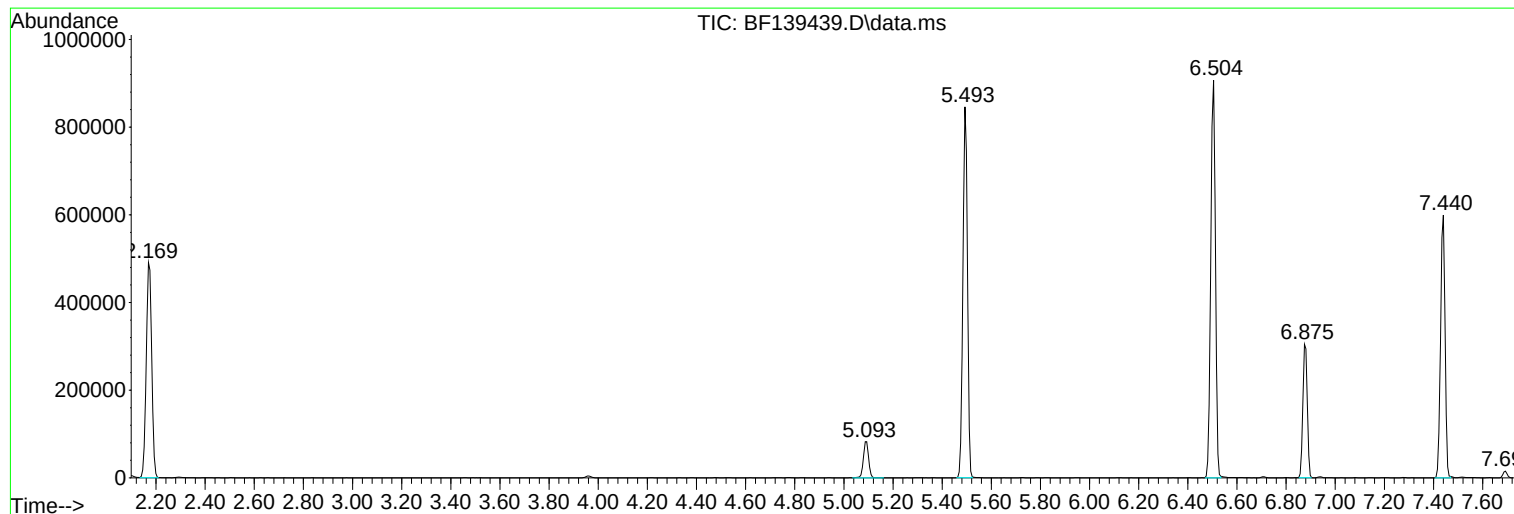
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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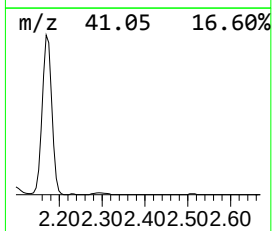
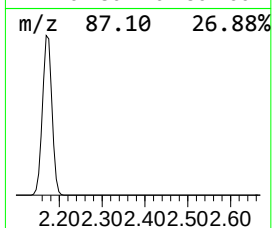
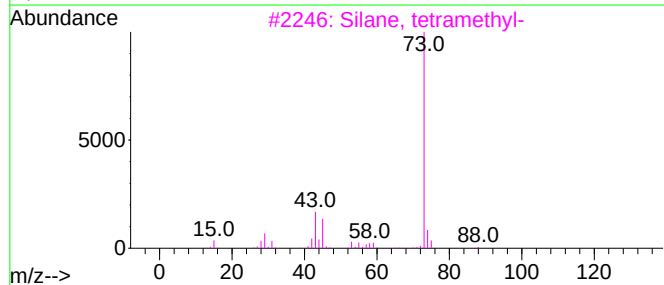
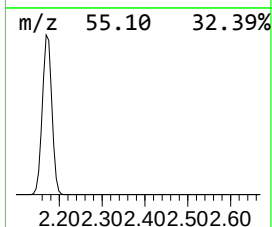
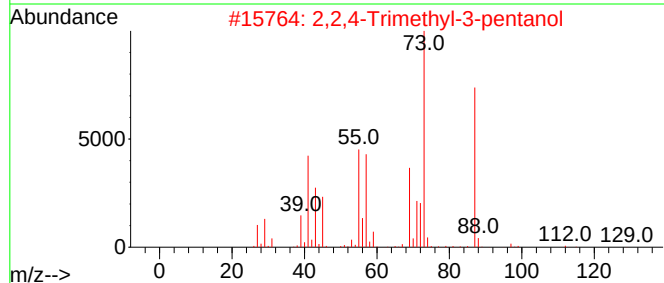
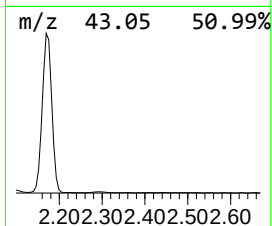
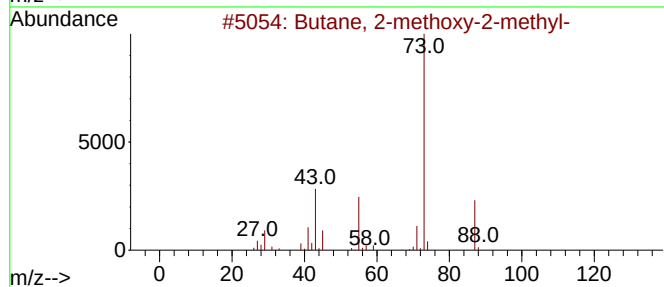
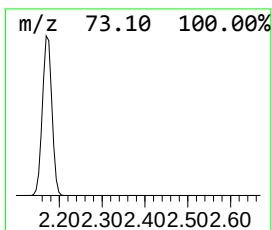
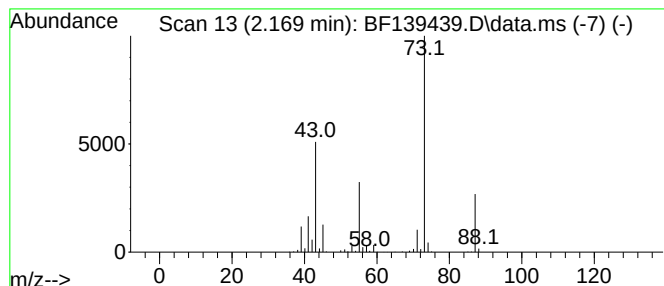
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.169	39.68 ng	755987	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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10
5			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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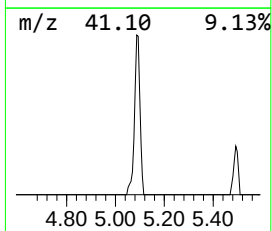
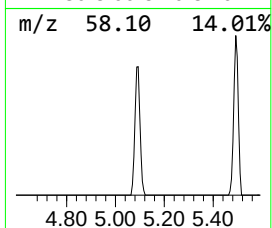
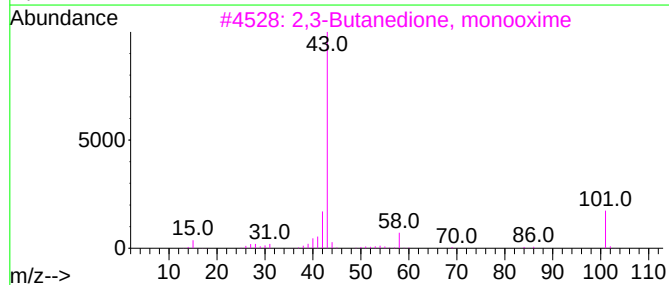
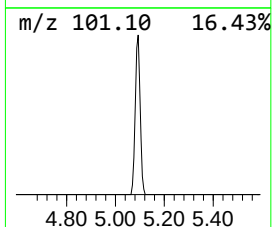
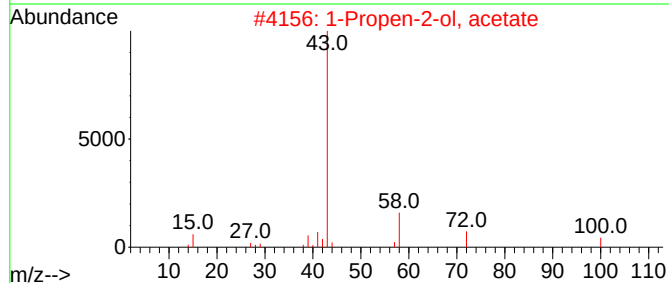
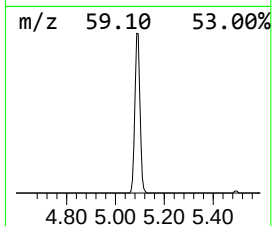
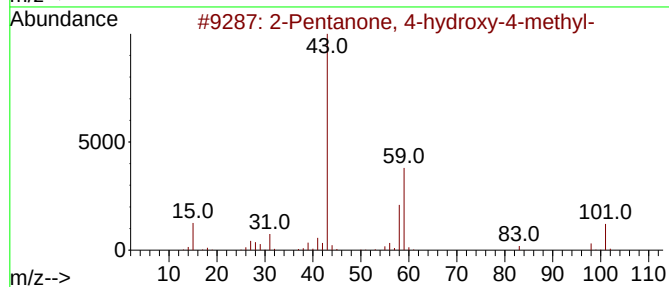
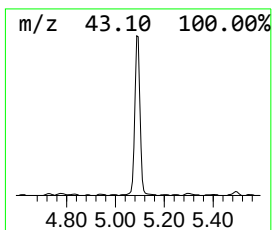
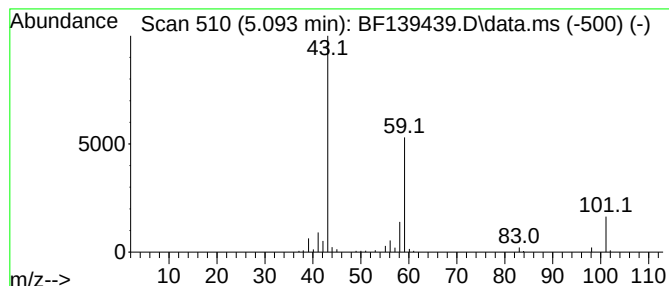
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	6.42 ng	122274	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	64
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Butane	58	C4H10	000106-97-8	9
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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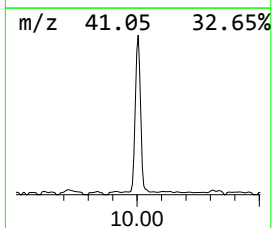
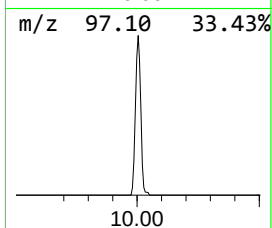
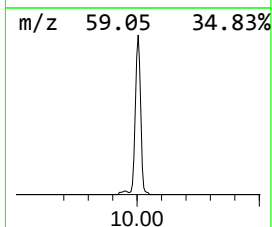
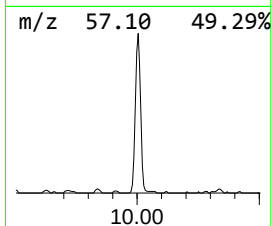
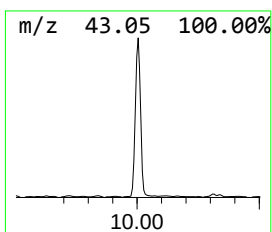
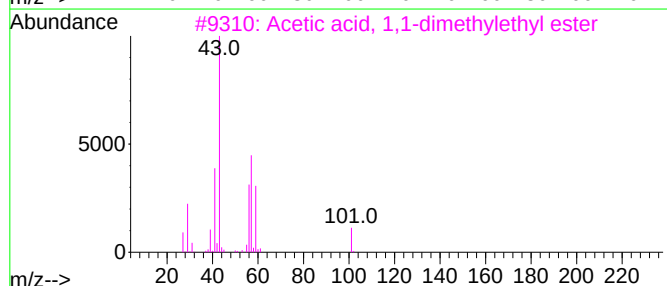
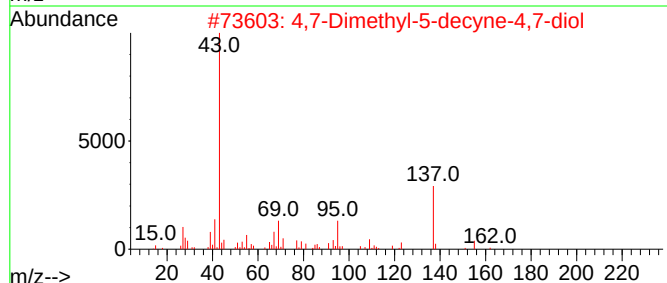
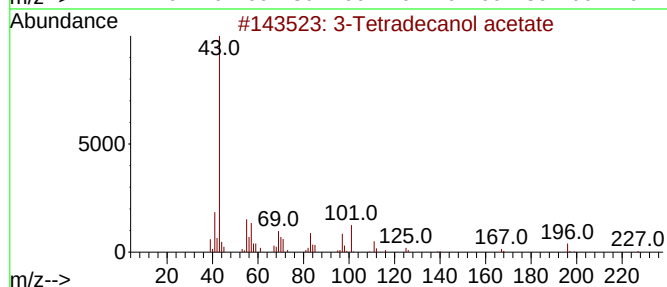
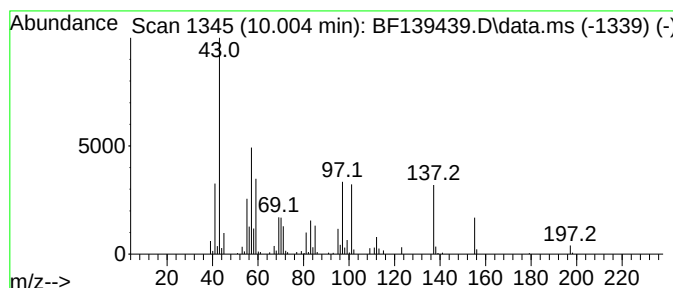
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.004 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.004	15.44 ng	319523	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Tetradecanol	acetate	256	C16H32O2	051354-23-5	25	
2	4,7-Dimethyl-5-decyne-4,7-diol	198	C12H22O2	000126-87-4	12		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10		
4	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	10		
5	(1S,2R,4R,7R)-4-Isopropyl-7-meth...	168	C10H16O2	001619-26-7	10		



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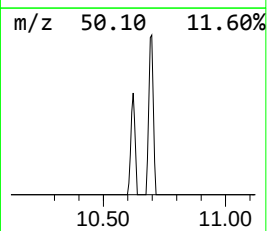
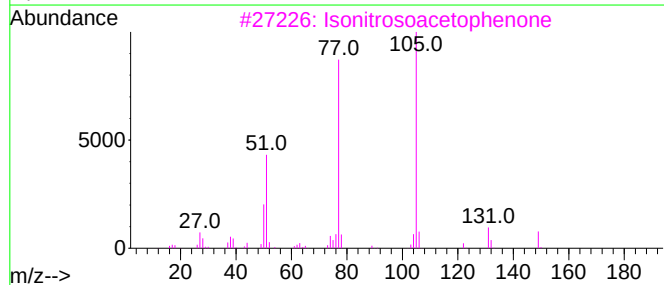
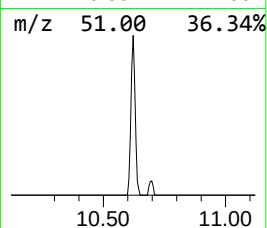
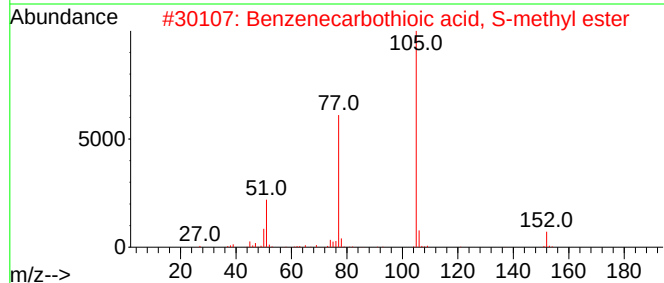
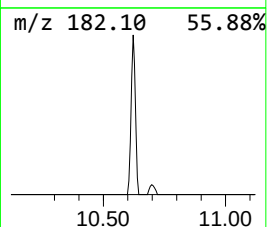
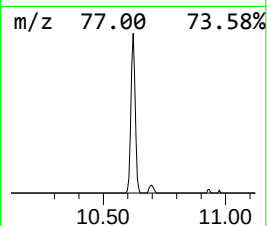
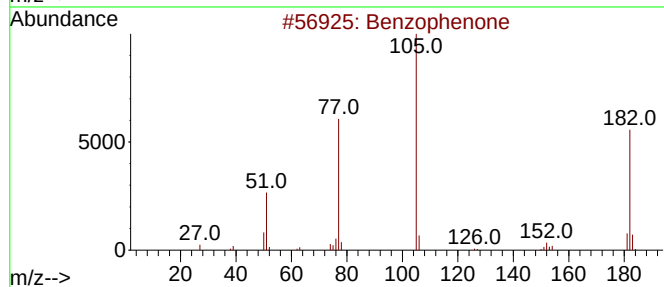
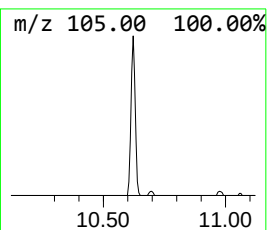
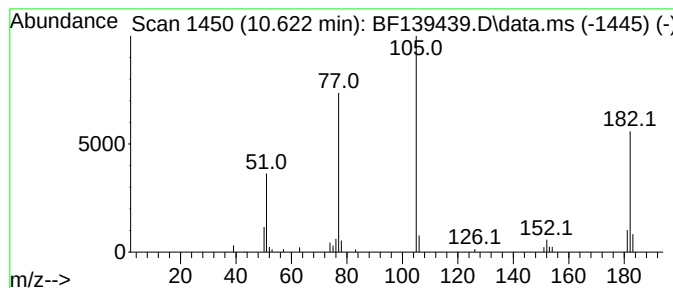
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	2.41 ng	49921	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	58
3			Isonitrosoacetophenone	149	C8H7NO2	000532-54-7	53
4			4,5-Diphenyloxazolin-2(3H)-one	237	C15H11NO2	005014-83-5	53
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	53



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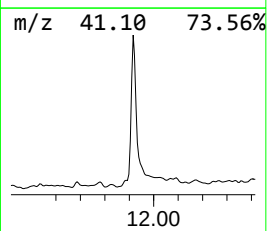
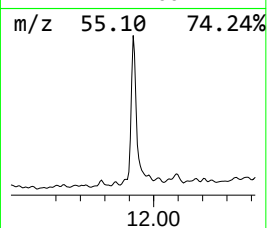
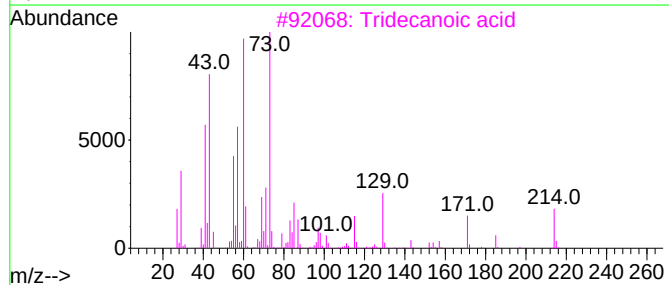
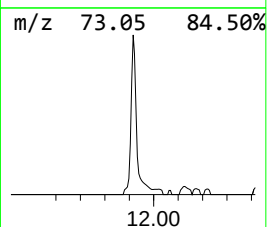
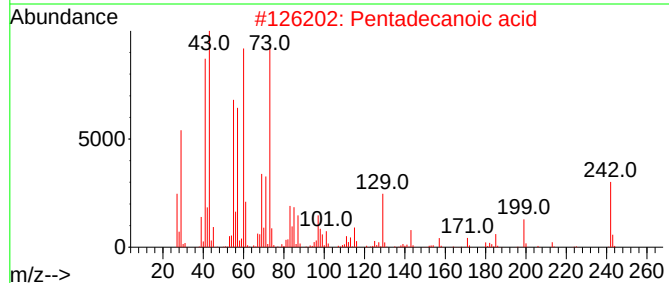
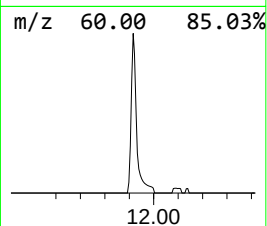
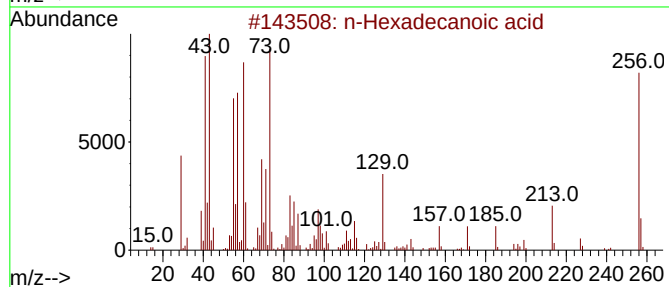
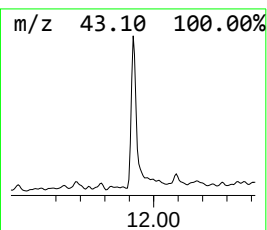
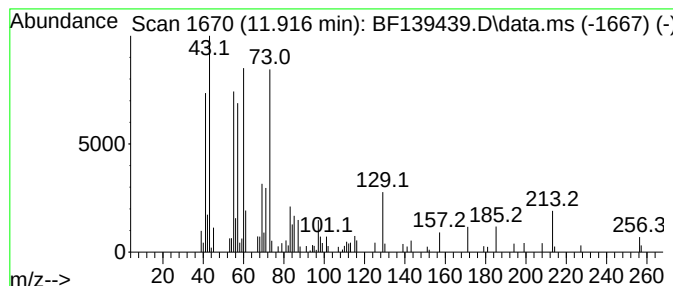
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	6.12 ng	124440	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tridecanoic acid	214	C13H26O2	000638-53-9	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139439.D
Acq On : 18 Sep 2024 21:41
Operator : RC/JU
Sample : P4087-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-614-COMP-01

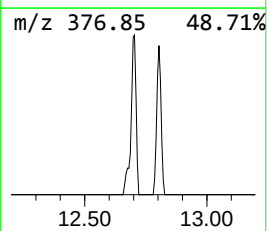
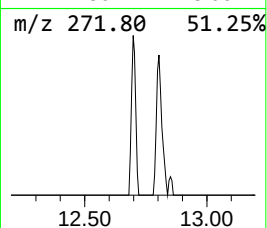
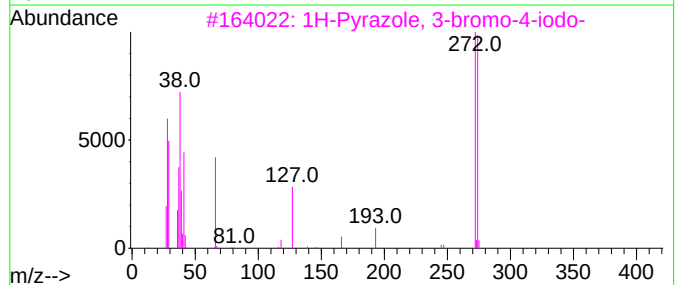
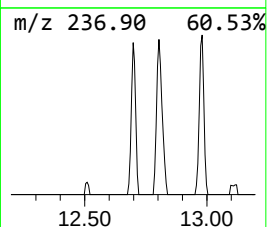
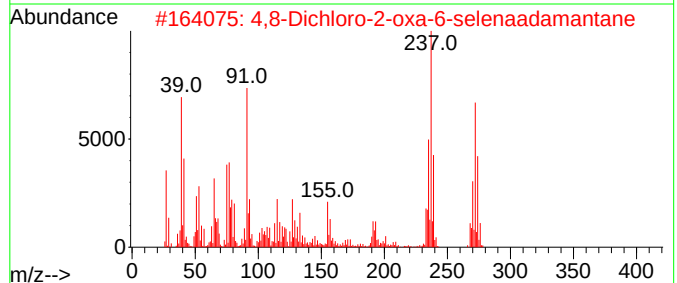
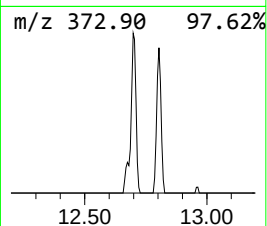
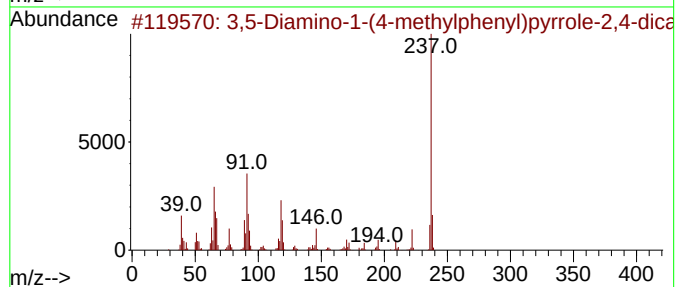
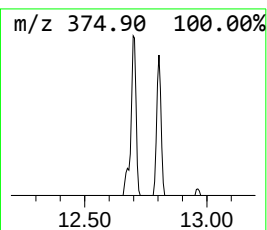
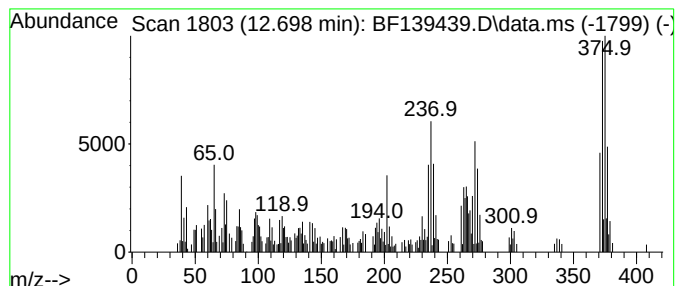
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.698 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	6.63 ng	134714	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5-Diamino-1-(4-methylphenyl)py...	237	C13H11N5	1000459-39-8	12
2			4,8-Dichloro-2-oxa-6-selenaadama...	272	C8H10Cl2OSe	1000189-96-4	10
3			1H-Pyrazole, 3-bromo-4-iodo-	272	C3H2BrIN2	1000460-68-5	10
4			4-Bromo-5-nitro-2H-pyrazole-3-ca...	235	C4H2BrN3O4	1000459-87-6	10
5			Monomethyltetrachloroterephthala...	388	C12H12Cl4O4Si	1000485-37-8	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139439.D
Acq On : 18 Sep 2024 21:41
Operator : RC/JU
Sample : P4087-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-614-COMP-01

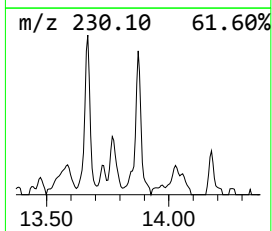
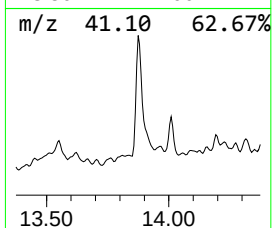
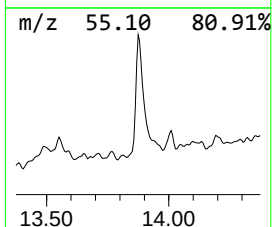
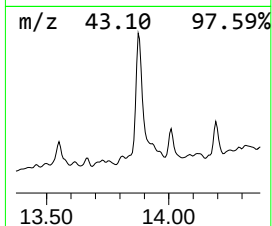
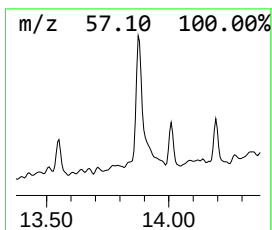
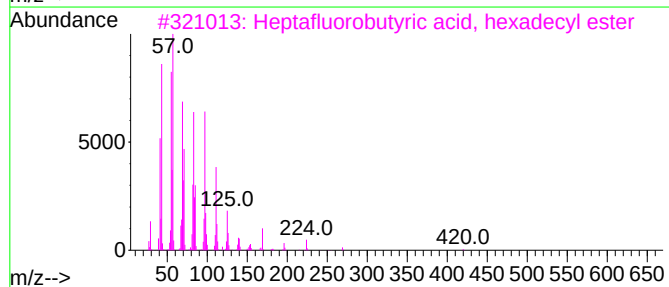
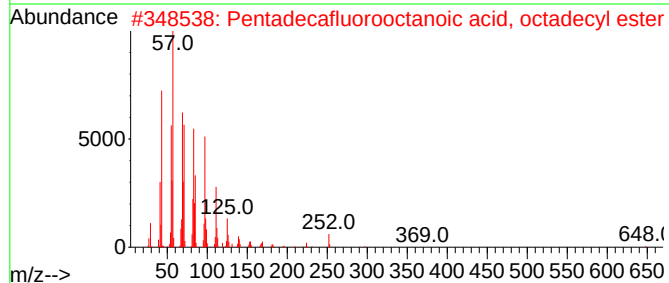
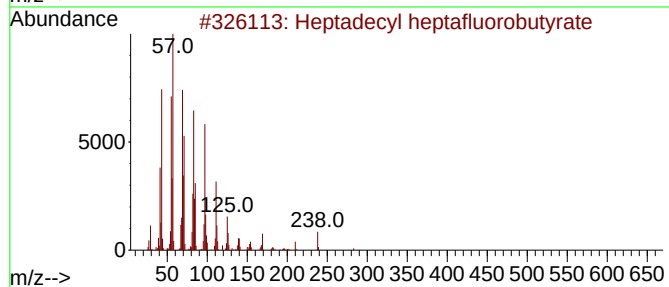
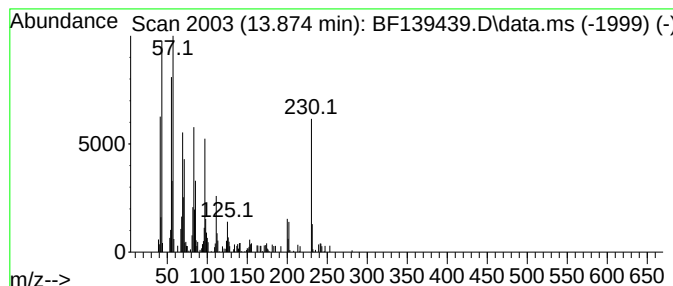
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	4.17 ng	100755	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	86
2		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	86
3		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	86
4		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	70
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139439.D
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Sample : P4087-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-614-COMP-01

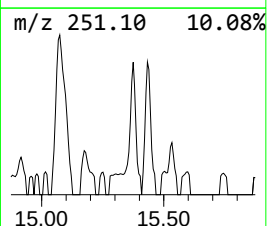
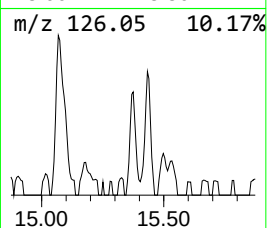
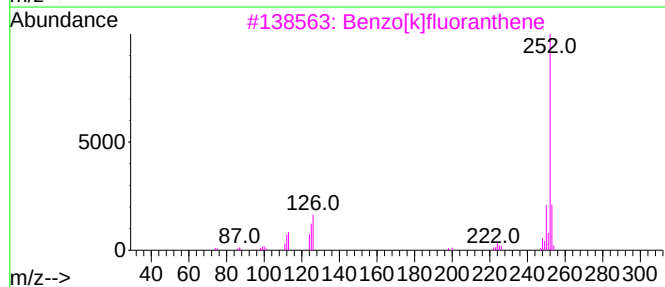
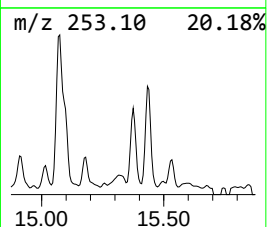
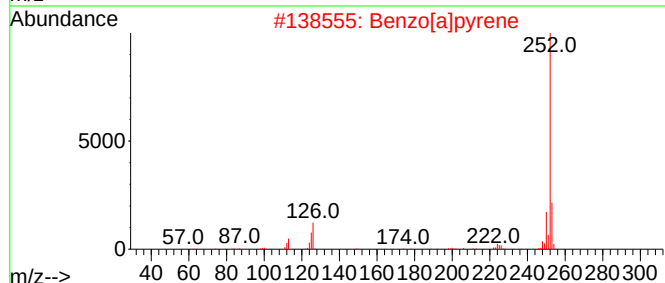
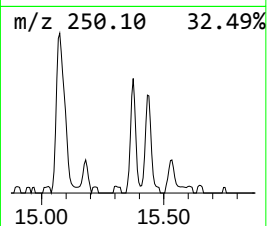
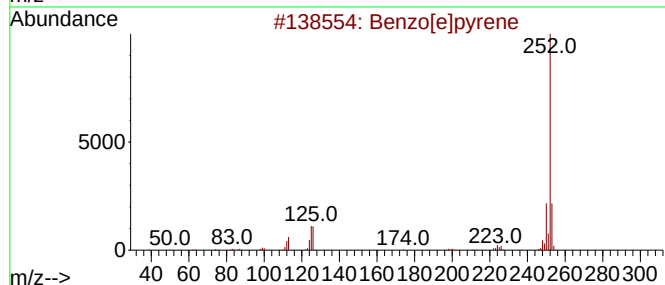
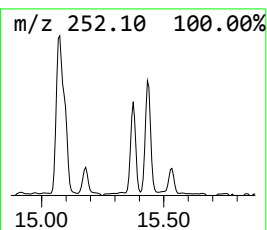
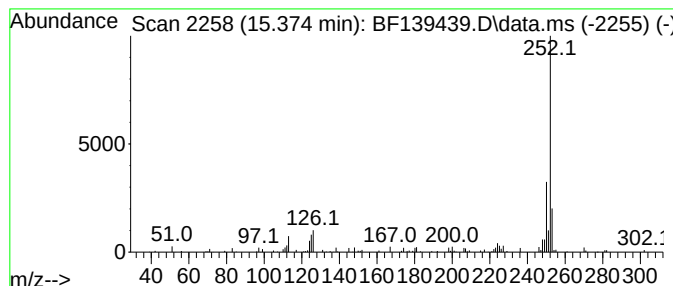
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	3.86 ng	44088	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	91
2			Benzo[a]pyrene	252	C20H12	000050-32-8	90
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	89
5			Perylene	252	C20H12	000198-55-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139439.D
Acq On : 18 Sep 2024 21:41
Operator : RC/JU
Sample : P4087-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-614-COMP-01

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	39.7	ng	755987	1	6.881	381083	20.0
2-Pentanone, 4-...	5.093	6.4	ng	122274	1	6.881	381083	20.0
unknown10.004	10.004	15.4	ng	319523	3	9.910	413762	20.0
Benzophenone	10.622	2.4	ng	49921	3	9.910	413762	20.0
n-Hexadecanoic ...	11.916	6.1	ng	124440	4	11.398	406343	20.0
unknown12.698	12.698	6.6	ng	134714	4	11.398	406343	20.0
Heptadecyl hept...	13.874	4.2	ng	100755	5	14.033	483542	20.0
Benzo[e]pyrene	15.374	3.9	ng	44088	6	15.498	228725	20.0