

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
 Data File : BF134586.D
 Acq On : 02 Aug 2023 18:33
 Operator : CG\JU
 Sample : 03842-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 342

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134586.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	6	14	22	rBV	65796	90164	2.23%	0.278%
2	5.028	490	500	509	rVB	96546	129799	3.21%	0.400%
3	5.422	562	567	570	rBV	3984810	3903504	96.62%	12.039%
4	6.428	732	738	740	rBV	3509851	3915283	96.91%	12.076%
5	6.622	768	771	777	rBV	119865	95118	2.35%	0.293%
6	6.792	797	800	804	rVB	1374770	1112725	27.54%	3.432%
7	7.357	890	896	898	rBV	2436056	2462759	60.96%	7.596%
8	8.069	1014	1017	1021	rBV	1595227	1434368	35.50%	4.424%
9	9.151	1196	1201	1204	rBV	4743377	4039919	100.00%	12.460%
10	9.269	1217	1221	1225	rVB	743833	625003	15.47%	1.928%
11	9.804	1308	1312	1313	rBV	415181	319811	7.92%	0.986%
12	9.828	1313	1316	1319	rVB	1595539	1333052	33.00%	4.111%
13	9.951	1331	1337	1341	rBV2	50217	48512	1.20%	0.150%
14	10.616	1445	1450	1453	rBV	2386317	2110177	52.23%	6.508%
15	11.316	1565	1569	1571	rBV	1281503	1188579	29.42%	3.666%
16	11.333	1571	1572	1576	rVB	198428	141454	3.50%	0.436%
17	11.386	1576	1581	1584	rVB	60051	54860	1.36%	0.169%
18	11.816	1650	1654	1656	rBV	69723	61761	1.53%	0.190%
19	11.851	1656	1660	1665	rVV2	422819	444995	11.01%	1.372%
20	11.927	1669	1673	1675	rBV2	56485	54977	1.36%	0.170%
21	12.051	1691	1694	1699	rVB2	78978	76932	1.90%	0.237%
22	12.369	1745	1748	1751	rBV	40618	45616	1.13%	0.141%
23	12.527	1771	1775	1778	rBV	345571	284723	7.05%	0.878%
24	12.639	1792	1794	1799	rVB2	102810	96204	2.38%	0.297%
25	12.727	1806	1809	1810	rBV2	70348	62654	1.55%	0.193%
26	12.757	1811	1814	1817	rVB	290331	259902	6.43%	0.802%
27	12.910	1836	1840	1843	rBV	3889381	3351060	82.95%	10.335%
28	13.086	1868	1870	1873	rVB	68498	55856	1.38%	0.172%
29	13.121	1873	1876	1879	rBV2	33730	49271	1.22%	0.152%
30	13.151	1879	1881	1884	rVV	67804	58737	1.45%	0.181%
31	13.186	1884	1887	1890	rVV2	56403	61146	1.51%	0.189%
32	13.680	1967	1971	1974	rBV	1595792	1293491	32.02%	3.989%
33	13.821	1992	1995	2002	rVB2	390547	415800	10.29%	1.282%
34	13.957	2013	2018	2021	rBV	1156163	1112626	27.54%	3.432%
35	13.980	2021	2022	2025	rVB	125206	89006	2.20%	0.275%
36	14.463	2101	2104	2113	rVB4	202435	272012	6.73%	0.839%

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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

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37	14.604	2125	2128	2132	rBV	138459	159162	3.94%	0.491%
38	14.992	2190	2194	2205	rVB	102897	217492	5.38%	0.671%
39	15.104	2210	2213	2215	rBV	57893	56767	1.41%	0.175%
40	15.292	2242	2245	2251	rVB	56161	74217	1.84%	0.229%
41	15.351	2252	2255	2260	rBV	57288	73701	1.82%	0.227%
42	15.421	2262	2267	2271	rBV	562838	689679	17.07%	2.127%

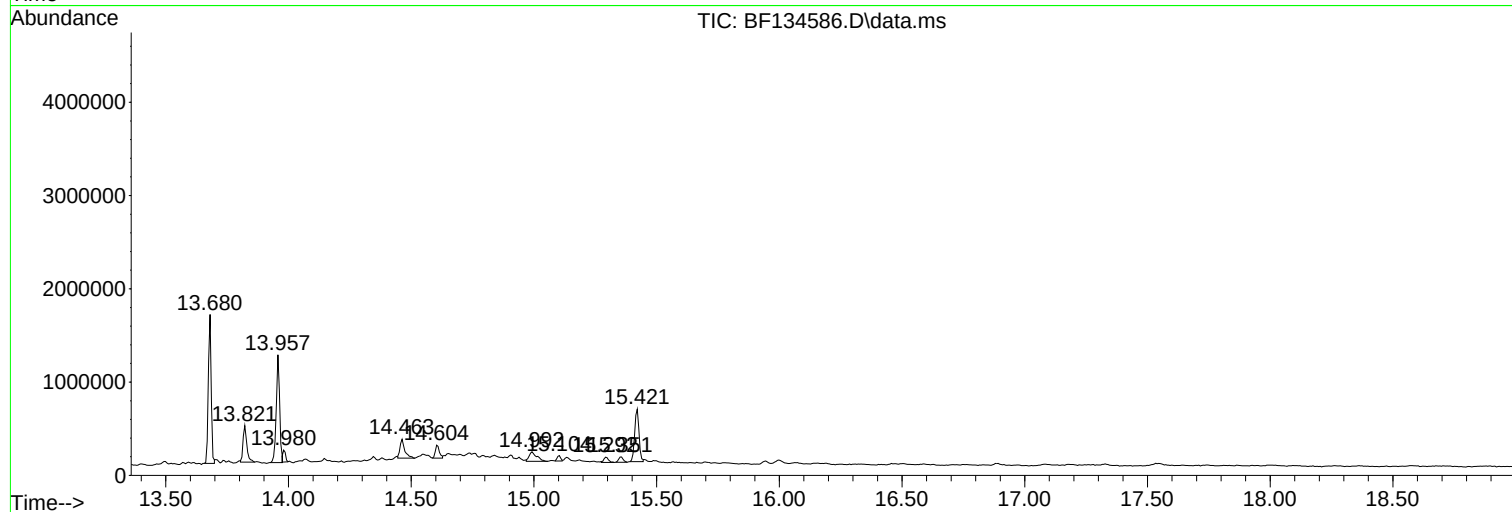
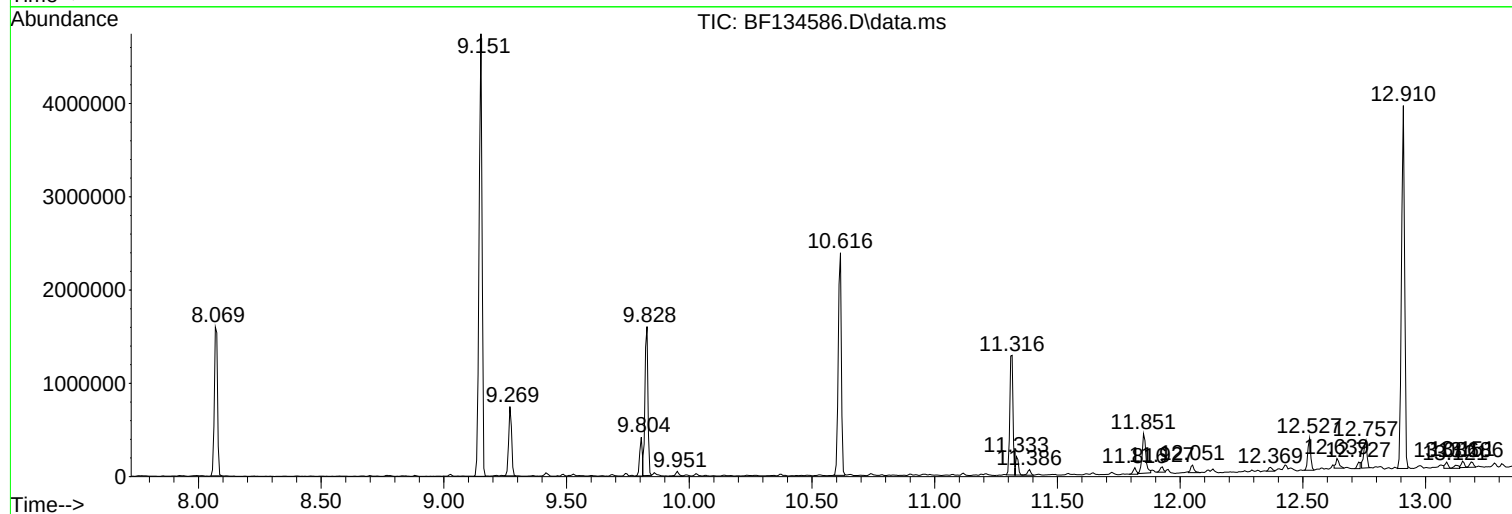
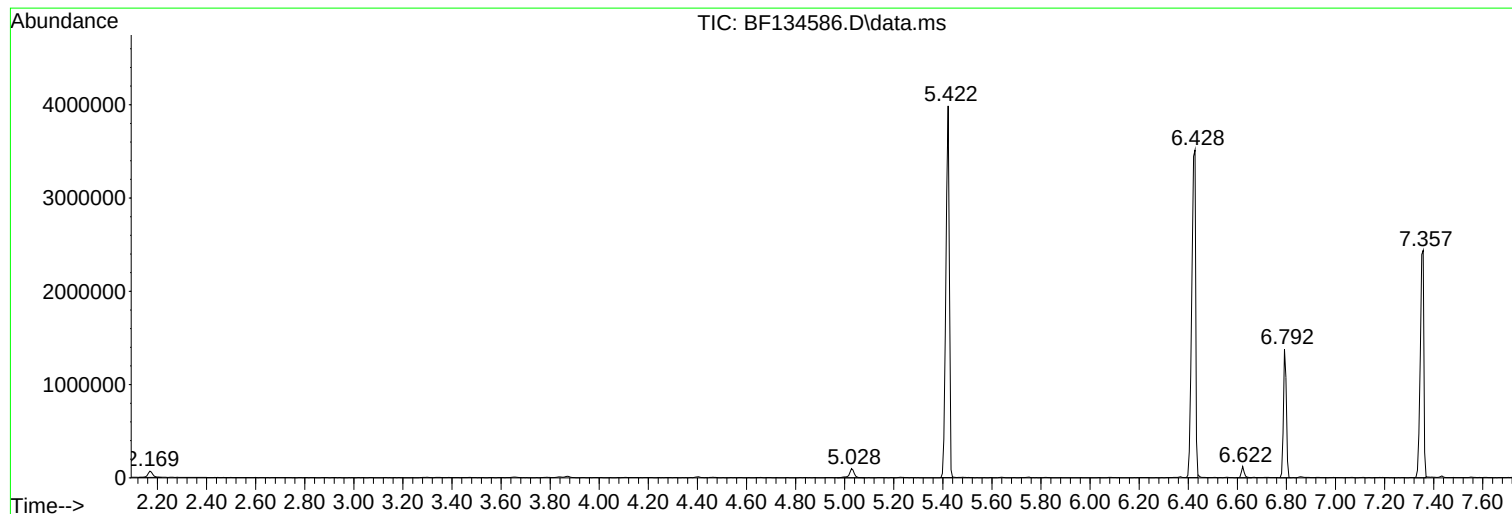
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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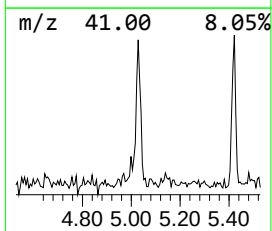
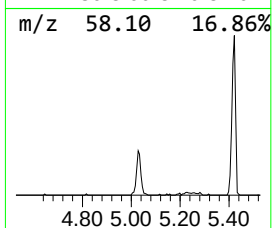
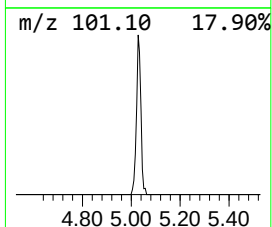
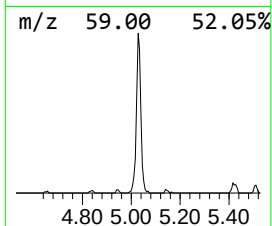
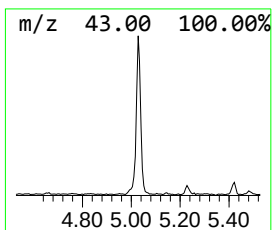
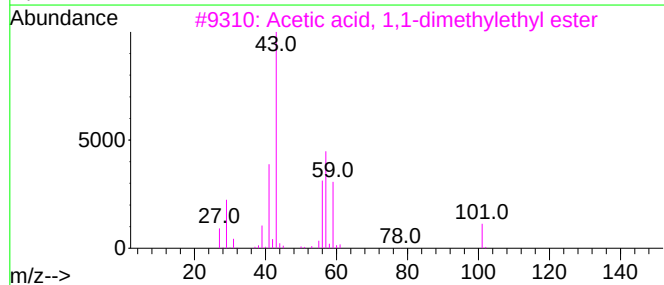
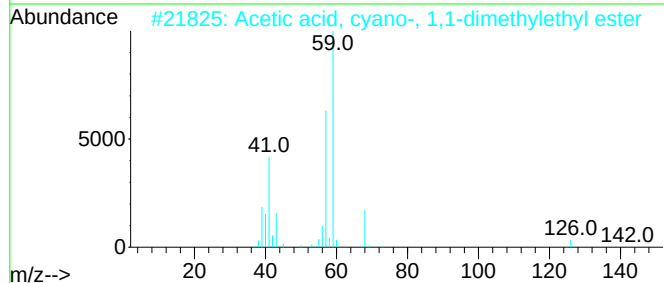
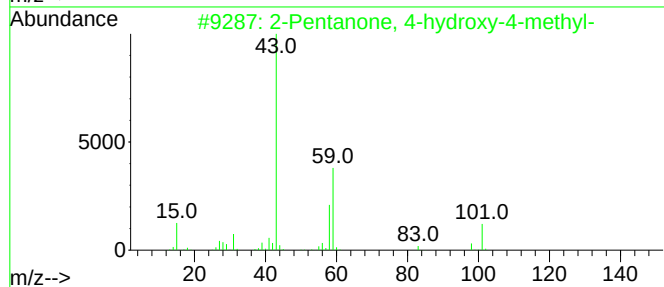
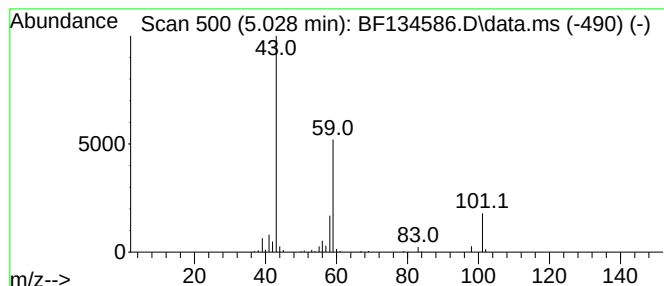
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	2.33 ng	129799	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10		



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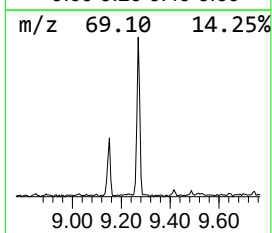
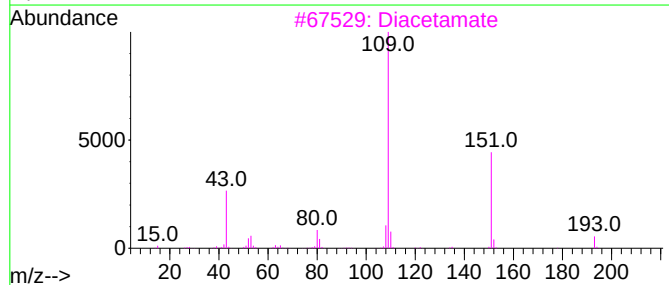
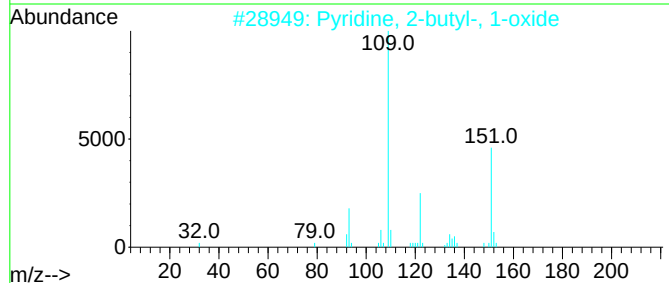
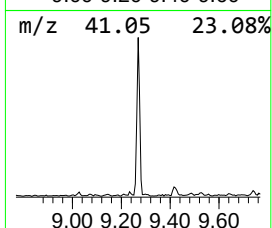
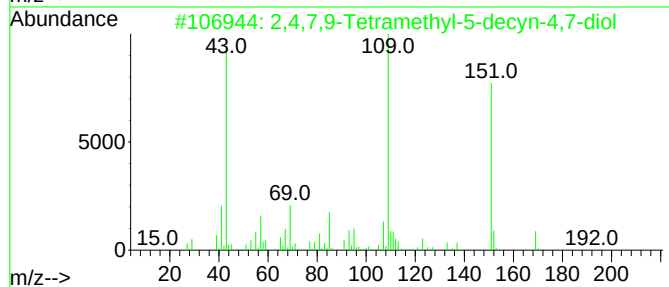
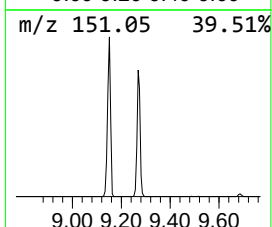
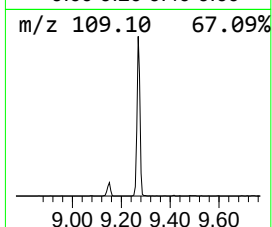
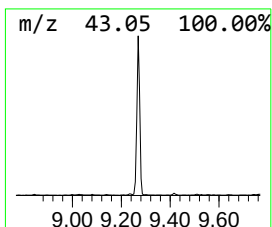
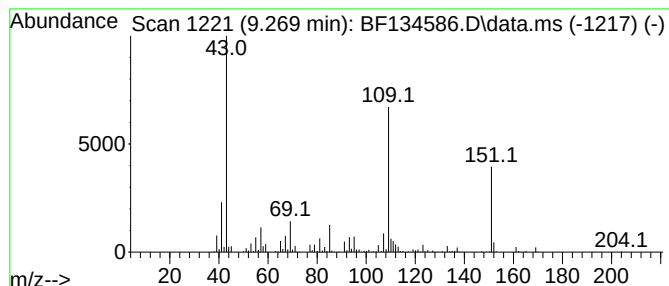
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.269	9.38 ng	625003	Acenaphthene-d10	9.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87	
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59	
3	Diacetamate	193	C10H11NO3	002623-33-8	53	
4	Acetaminophen	151	C8H9NO2	000103-90-2	53	
5	Metacetamol	151	C8H9NO2	000621-42-1	53	



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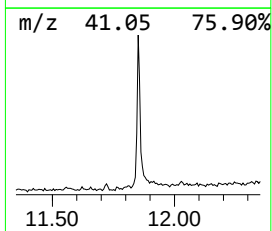
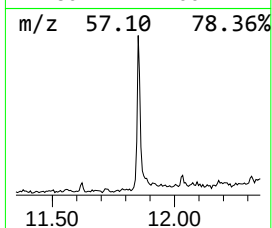
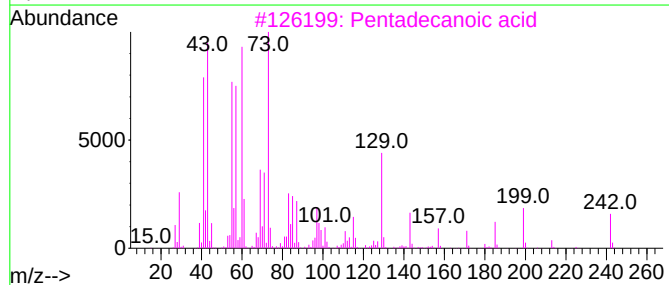
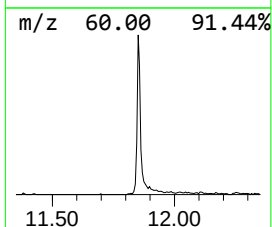
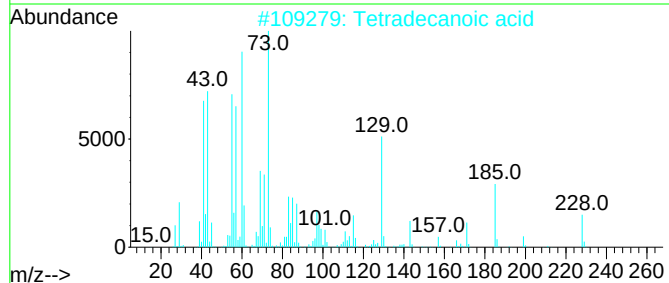
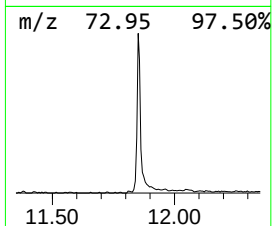
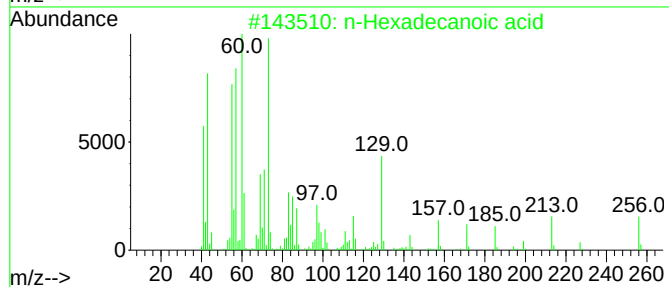
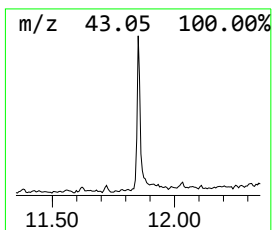
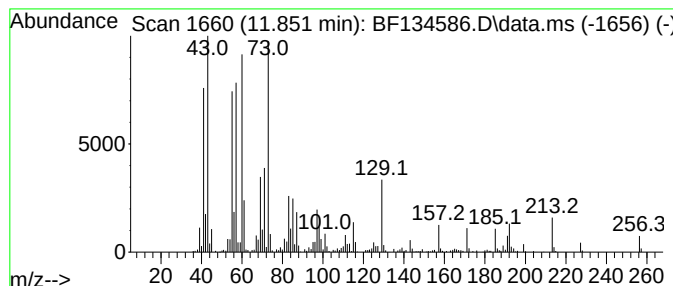
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	7.49 ng	444995	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	87
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	53



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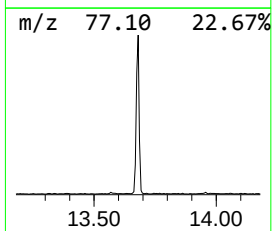
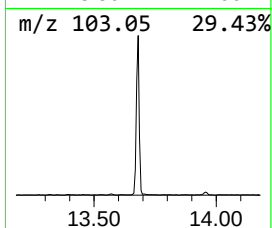
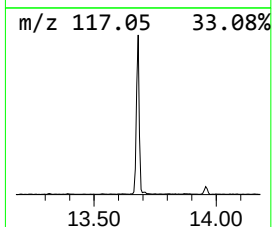
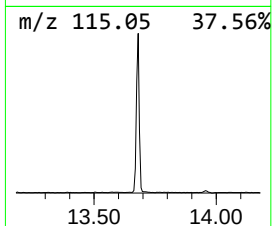
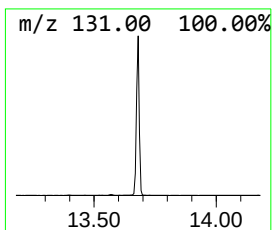
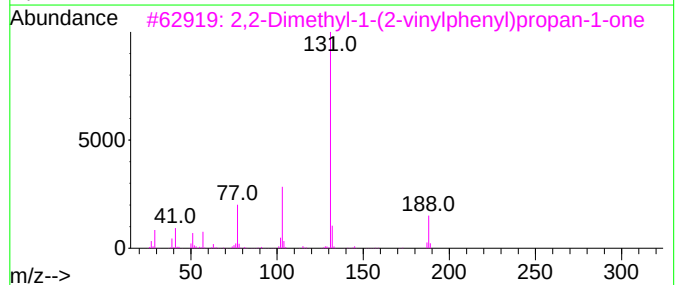
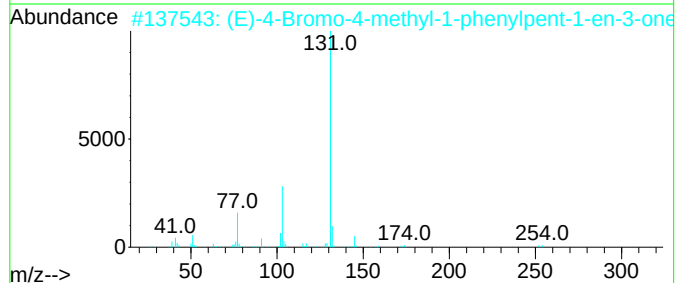
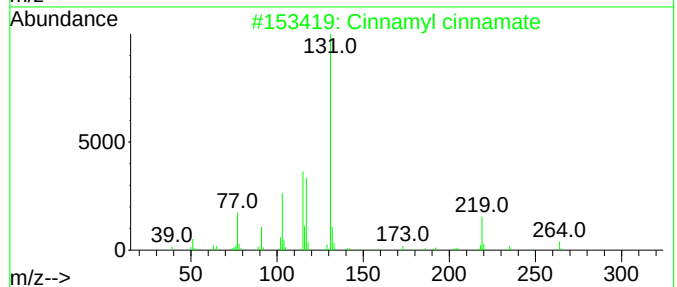
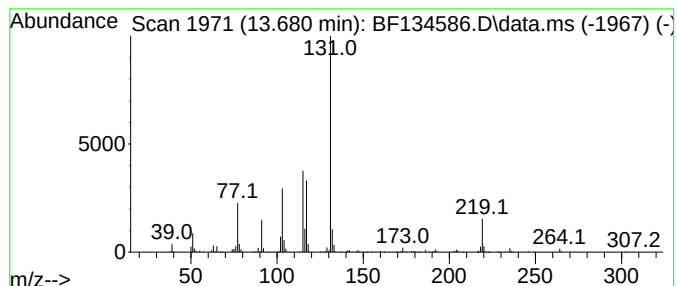
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.680	23.25 ng	1293490	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	53
3			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
4			N-(4-Fluorophenyl)-3-phenyl-2-pr...	337	C17H11F4NO2	1000492-37-5	50
5			1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	50



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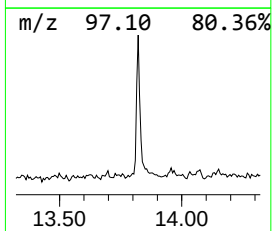
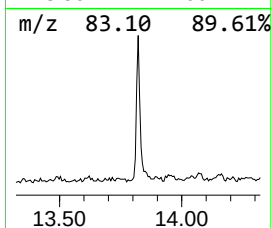
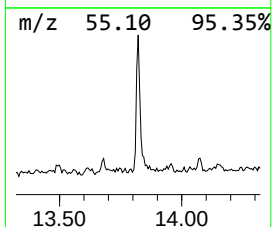
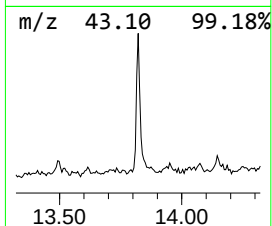
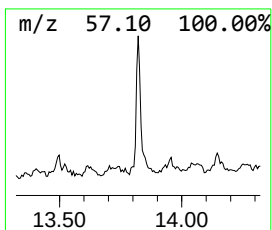
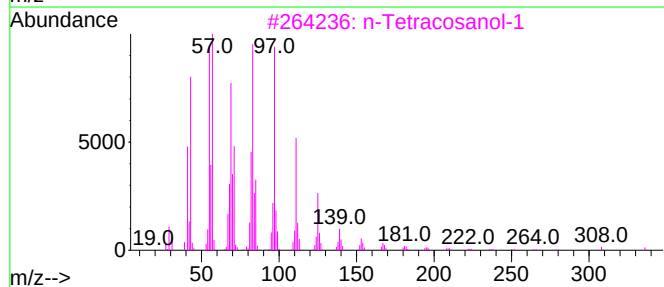
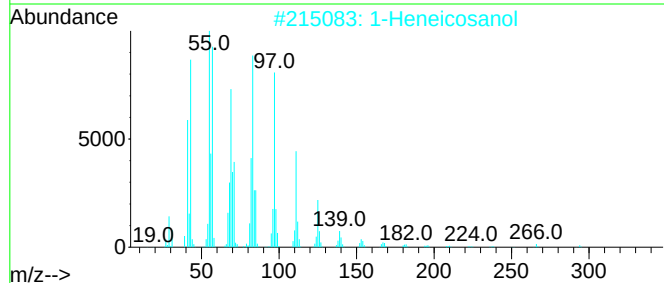
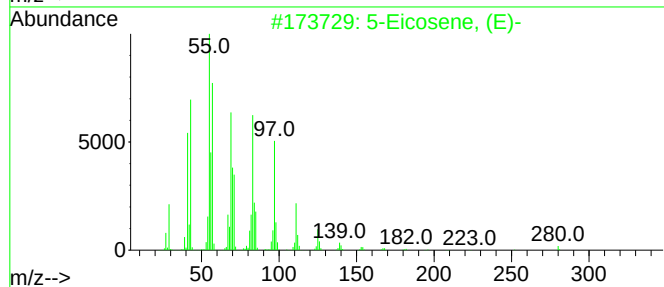
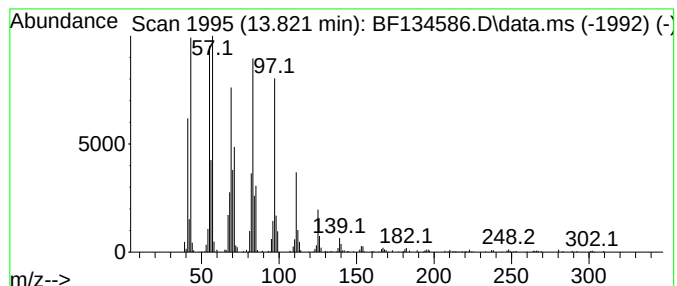
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	7.47 ng	415800	Chrysene-d12	13.957

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		1-Heneicosanol	312	C21H44O	015594-90-8	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134586.D
Acq On : 02 Aug 2023 18:33
Operator : CG\JU
Sample : 03842-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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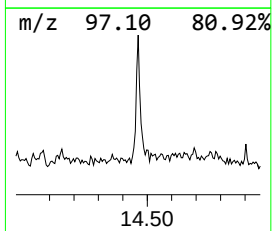
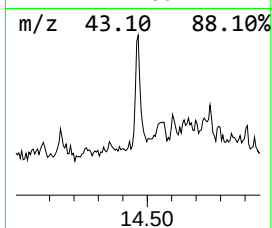
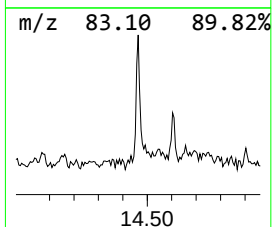
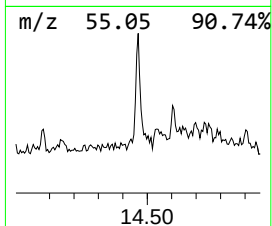
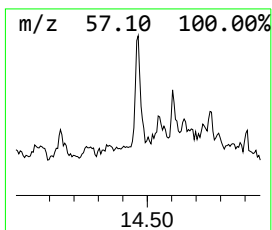
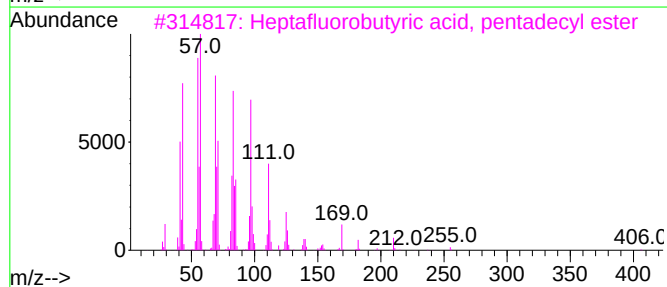
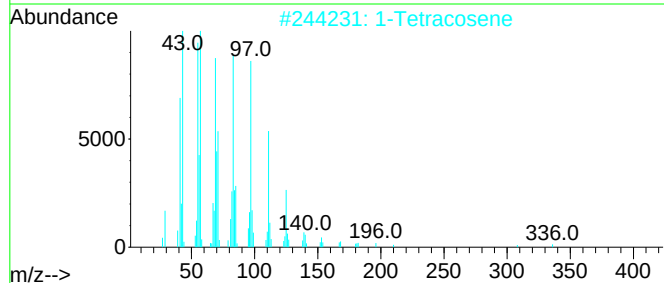
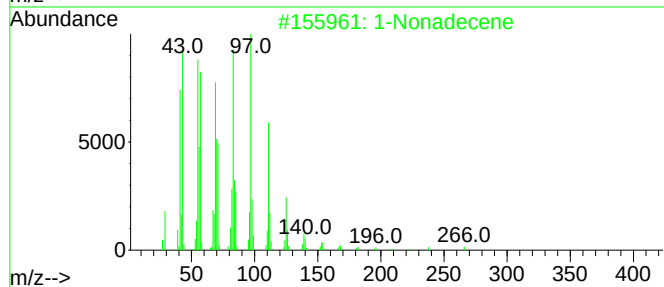
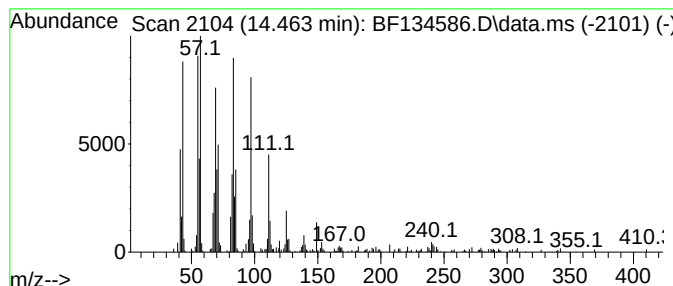
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.463	4.89 ng	272012	Chrysene-d12	13.957

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Nonadecene	266	C19H38	018435-45-5	97
2		1-Tetracosene	336	C24H48	010192-32-2	94
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4		Nonacos-1-ene	406	C29H58	018835-35-3	94
5		1-Tricosene	322	C23H46	018835-32-0	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134586.D
Acq On : 02 Aug 2023 18:33
Operator : CG\JU
Sample : 03842-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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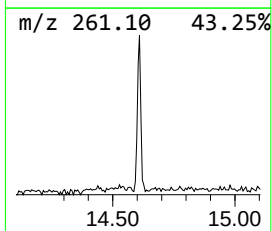
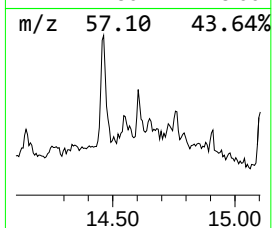
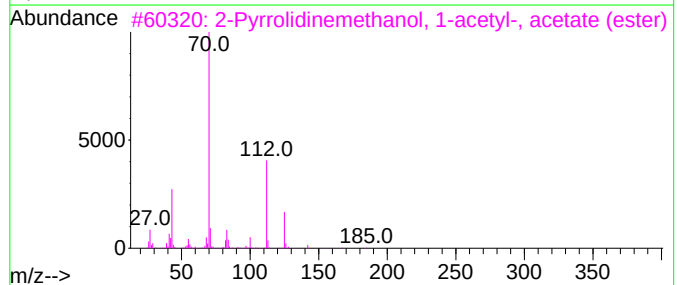
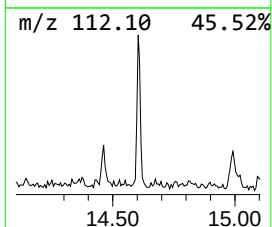
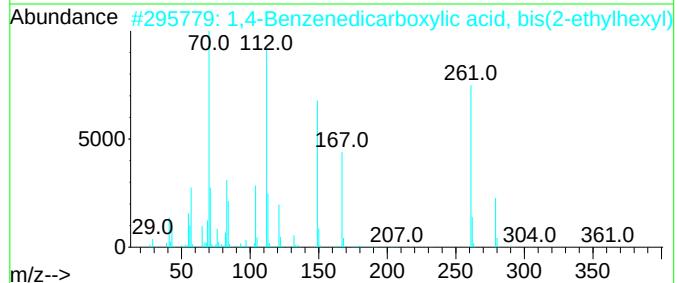
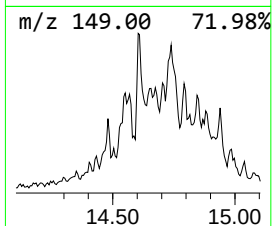
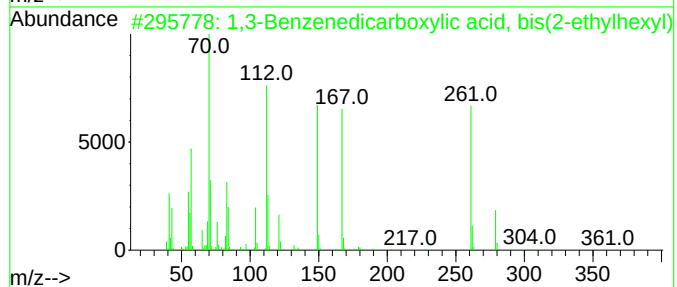
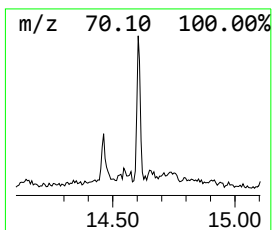
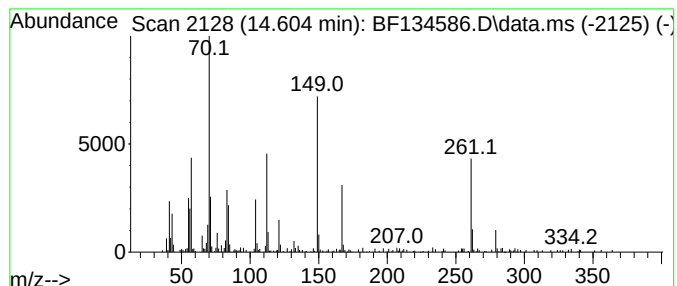
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,3-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.604	2.86 ng	159162	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	80
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	74
3			2-Pyrrolidinemethanol, 1-acetyl-...	185	C9H15NO3	042366-60-9	27
4			1-(2-Hydroxymethylpyrrolidin-1-y...	143	C7H13NO2	1000192-83-2	27
5			Pyrrolidin-1-yl phenyl ketoxime	190	C11H14N2O	1000144-18-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134586.D
Acq On : 02 Aug 2023 18:33
Operator : CG\JU
Sample : 03842-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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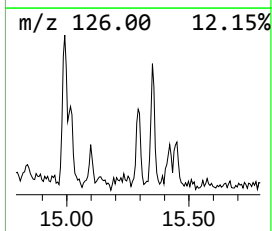
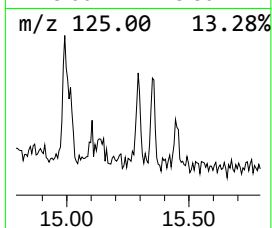
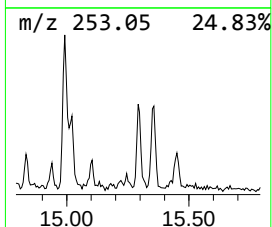
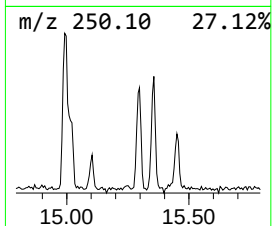
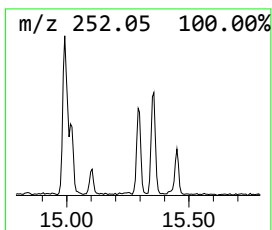
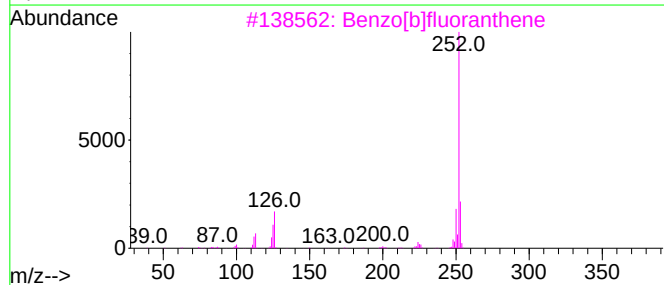
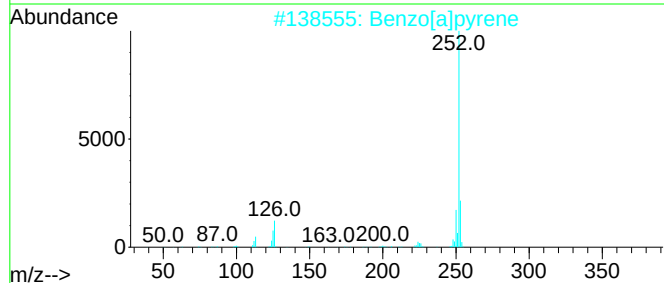
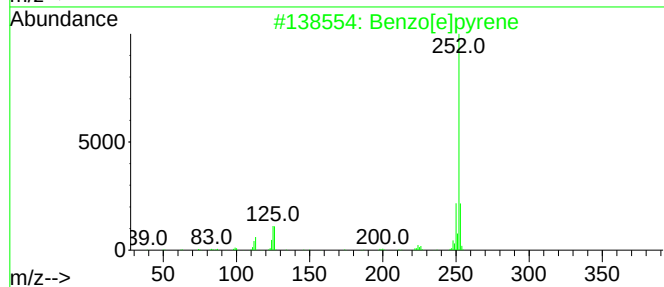
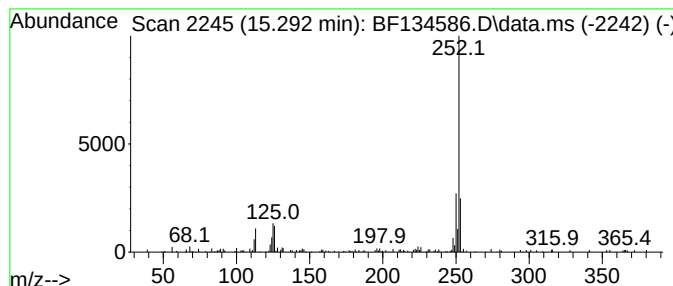
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	2.15 ng	74217	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	94
2			Benzo[a]pyrene	252	C20H12	000050-32-8	94
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
5			Perylene	252	C20H12	000198-55-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134586.D
Acq On : 02 Aug 2023 18:33
Operator : CG\JU
Sample : 03842-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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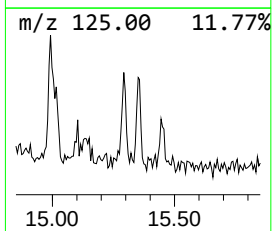
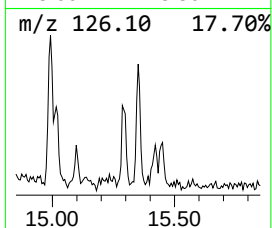
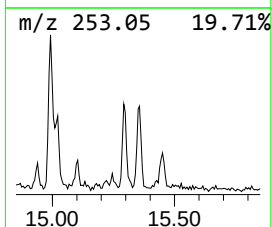
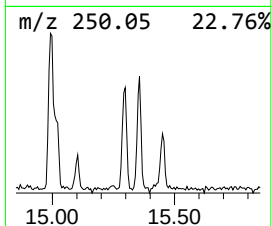
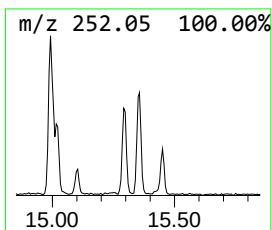
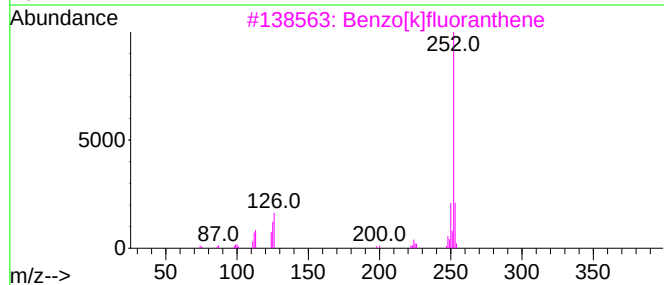
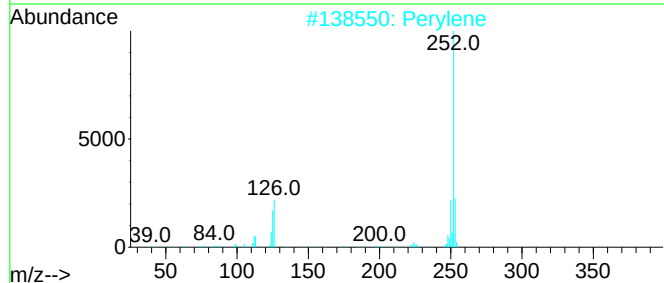
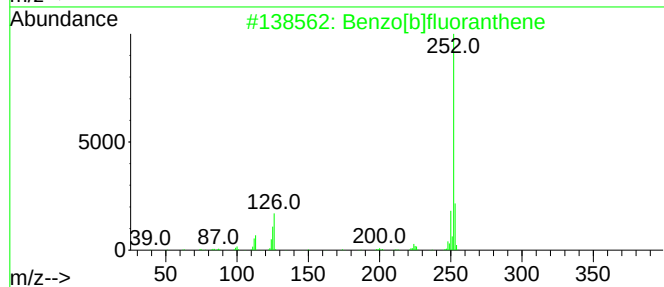
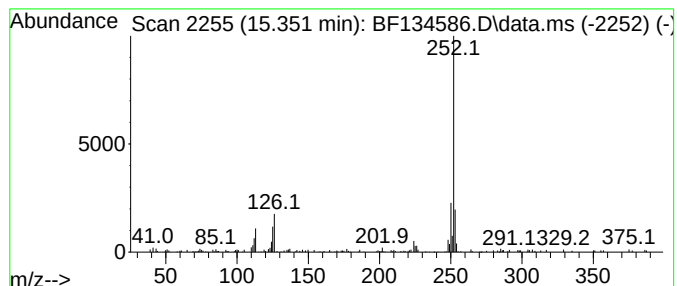
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	2.14 ng	73701	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
2			Perylene	252	C20H12	000198-55-0	93
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[e]pyrene	252	C20H12	000192-97-2	91
5			Benzo[a]pyrene	252	C20H12	000050-32-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134586.D
Acq On : 02 Aug 2023 18:33
Operator : CG\JU
Sample : 03842-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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
2-Pentanone, 4-...	5.028	2.3	ng	129799	1	6.792	1112730	20.0
2,4,7,9-Tetrame...	9.269	9.4	ng	625003	3	9.828	1333050	20.0
n-Hexadecanoic ...	11.851	7.5	ng	444995	4	11.316	1188580	20.0
Cinnamyl cinnamate	13.680	23.3	ng	1293490	5	13.957	1112630	20.0
5-Eicosene, (E)-	13.821	7.5	ng	415800	5	13.957	1112630	20.0
1-Nonadecene	14.463	4.9	ng	272012	5	13.957	1112630	20.0
1,3-Benzenedica...	14.604	2.9	ng	159162	5	13.957	1112630	20.0
Benzo[e]pyrene	15.292	2.1	ng	74217	6	15.421	689679	20.0
Perylene	15.351	2.1	ng	73701	6	15.421	689679	20.0