

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
 Data File : BF126578.D
 Acq On : 10 Jan 2022 20:35
 Operator : JU/CG
 Sample : N1080-02
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 289

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-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126578.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.993	491	494	505	rVB	58407	78079	3.11%	0.400%
2	5.392	557	562	565	rBV	2416480	2477347	98.77%	12.680%
3	6.410	729	735	738	rBV	2243000	2508078	100.00%	12.837%
4	6.769	792	796	799	rBV	668996	527592	21.04%	2.700%
5	7.334	886	892	895	rBV	1593037	1688917	67.34%	8.644%
6	7.957	994	998	1006	rBV	171539	149623	5.97%	0.766%
7	8.051	1010	1014	1017	rBV	832916	707428	28.21%	3.621%
8	9.133	1192	1198	1201	rBV	2480992	2322184	92.59%	11.886%
9	9.810	1308	1313	1316	rBV	759084	693983	27.67%	3.552%
10	9.839	1316	1318	1321	rVB	36467	26295	1.05%	0.135%
11	10.598	1440	1447	1450	rBV	1486901	1292611	51.54%	6.616%
12	11.292	1561	1565	1567	rBV	691012	565575	22.55%	2.895%
13	11.316	1567	1569	1572	rVV	208111	158717	6.33%	0.812%
14	11.369	1575	1578	1582	rVB	41018	36041	1.44%	0.184%
15	11.527	1600	1605	1611	rBV2	15788	25265	1.01%	0.129%
16	11.798	1648	1651	1654	rBV2	19644	28628	1.14%	0.147%
17	11.833	1654	1657	1662	rVV2	84120	91118	3.63%	0.466%
18	11.910	1667	1670	1672	rBV	33894	32094	1.28%	0.164%
19	12.280	1730	1733	1741	rBV5	19955	42947	1.71%	0.220%
20	12.345	1741	1744	1756	rBV	1609344	1781324	71.02%	9.117%
21	12.510	1768	1772	1775	rVB	247420	221959	8.85%	1.136%
22	12.621	1788	1791	1795	rBV	68866	78138	3.12%	0.400%
23	12.663	1795	1798	1802	rVB	60762	63261	2.52%	0.324%
24	12.733	1805	1810	1813	rBV	226173	243626	9.71%	1.247%
25	12.886	1832	1836	1839	rVB	1659142	1464387	58.39%	7.495%
26	12.945	1844	1846	1852	rVB4	38917	51880	2.07%	0.266%
27	13.068	1862	1867	1869	rVB2	42267	60978	2.43%	0.312%
28	13.133	1870	1878	1881	rBV4	30585	62072	2.47%	0.318%
29	13.192	1886	1888	1892	rVB5	23825	28366	1.13%	0.145%
30	13.263	1898	1900	1903	rVB2	33479	33098	1.32%	0.169%
31	13.792	1987	1990	1998	rVB2	130459	180389	7.19%	0.923%
32	13.939	2010	2015	2018	rBV2	539308	591416	23.58%	3.027%
33	13.963	2018	2019	2025	rVB	97550	68354	2.73%	0.350%
34	14.039	2028	2032	2037	rBV2	82961	103192	4.11%	0.528%
35	14.427	2096	2098	2102	rBV3	39174	48060	1.92%	0.246%
36	14.592	2123	2126	2129	rBV2	35065	44738	1.78%	0.229%

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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-BF122921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.980	2189	2192	2200	rVB	114238	221487	8.83%	1.134%
38	15.274	2239	2242	2248	rVB	68282	91795	3.66%	0.470%
39	15.333	2249	2252	2258	rVB	88134	102362	4.08%	0.524%
40	15.398	2258	2263	2267	rBV	372561	468516	18.68%	2.398%
41	16.809	2500	2503	2515	rVB2	34939	76023	3.03%	0.389%

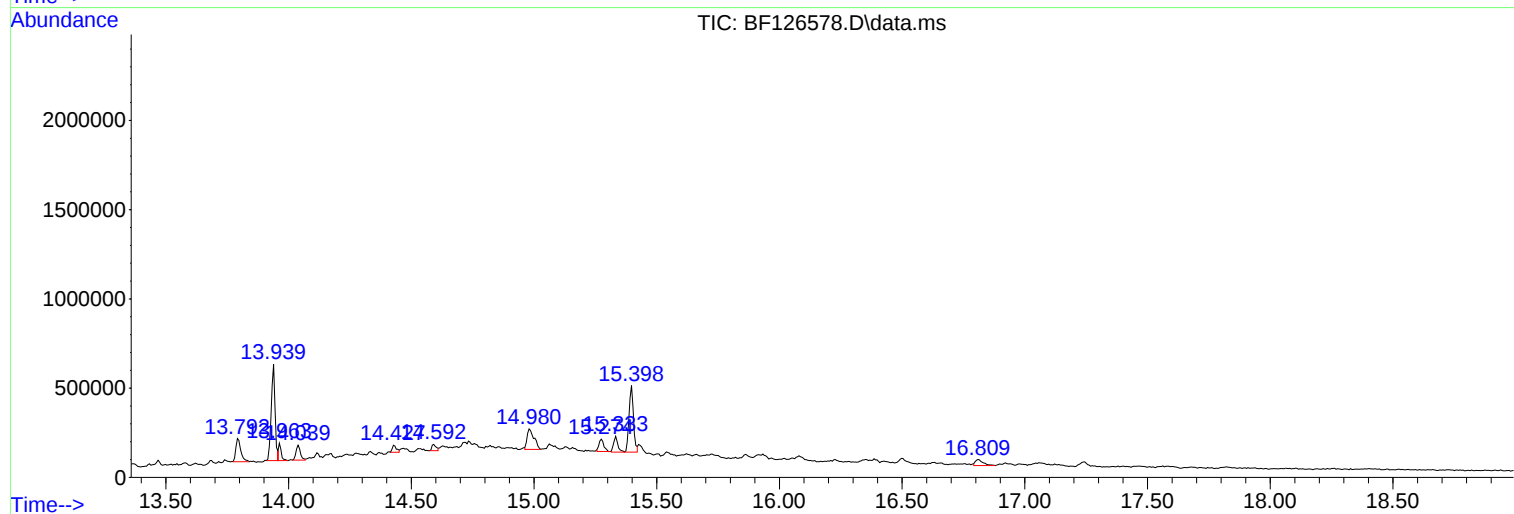
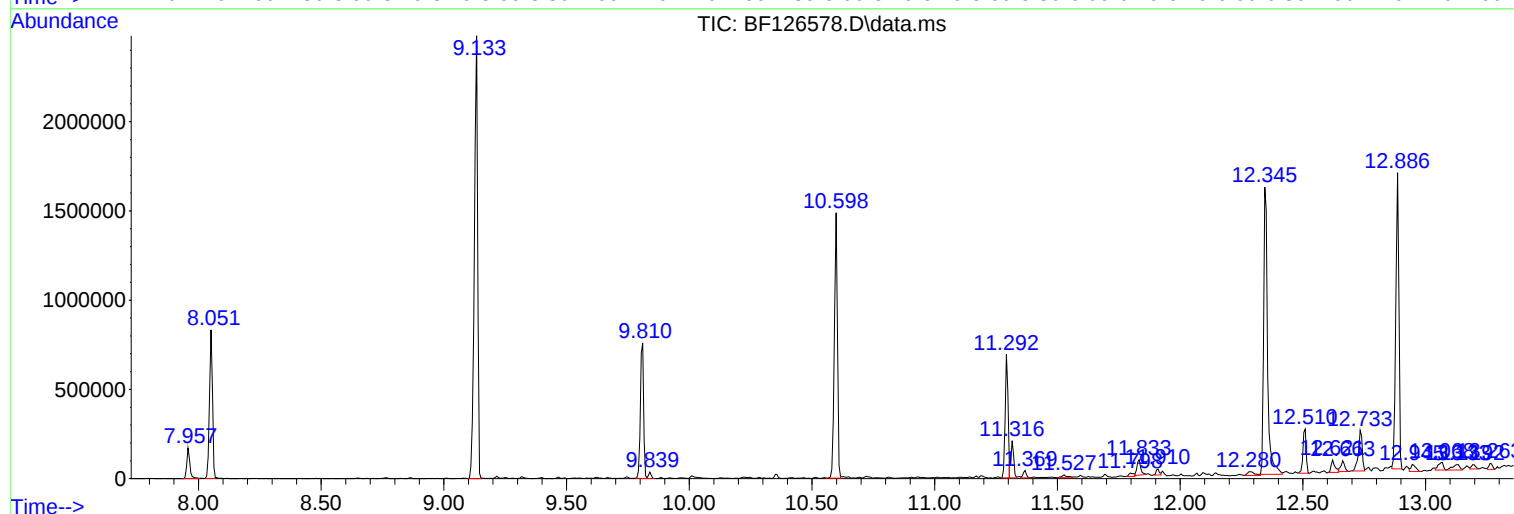
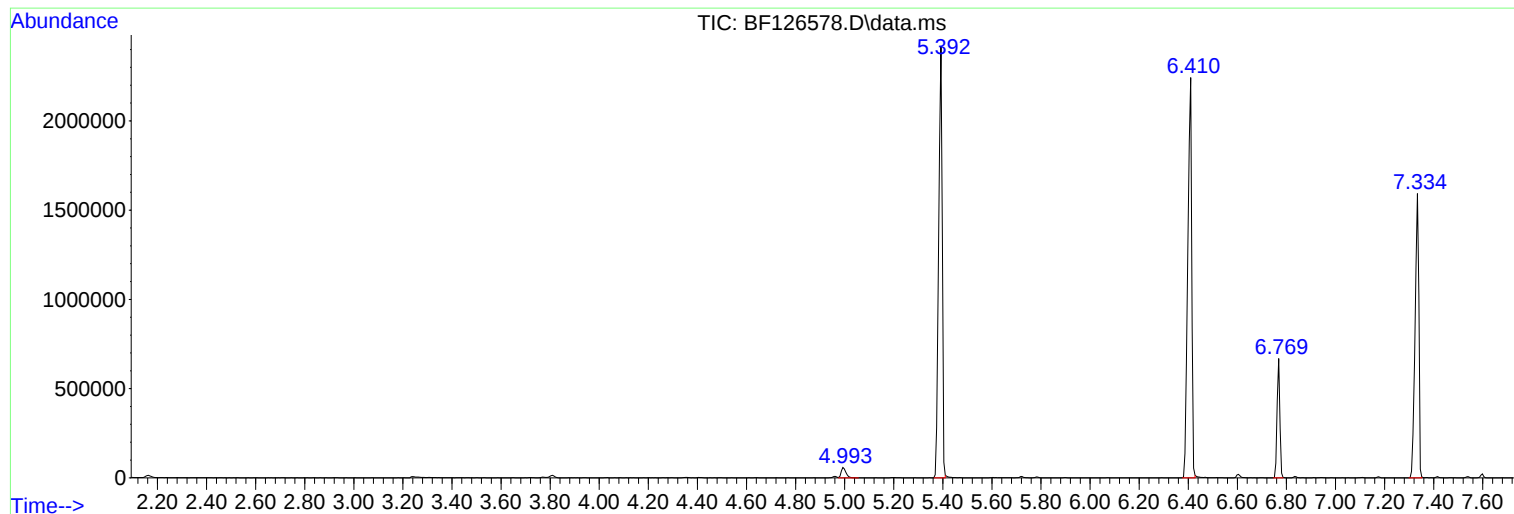
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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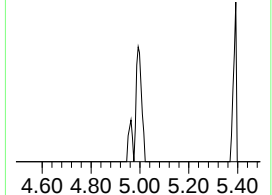
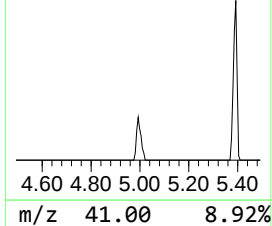
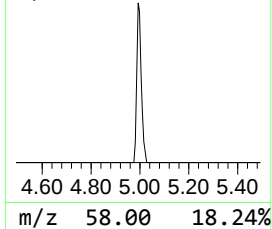
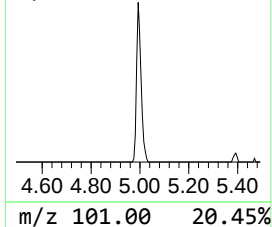
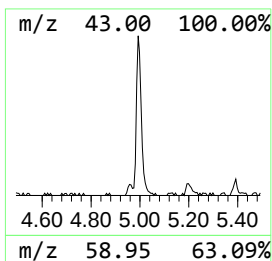
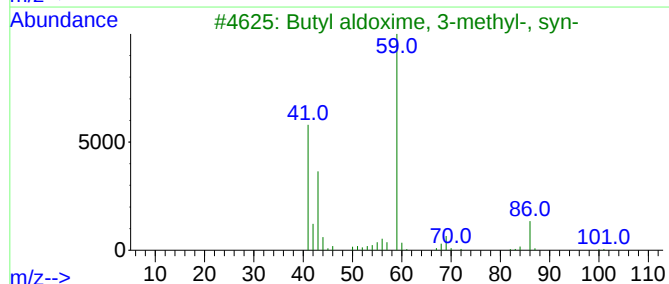
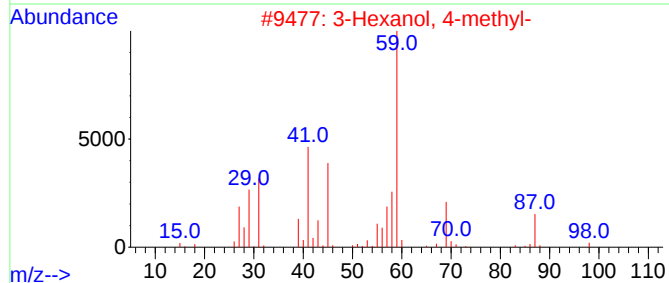
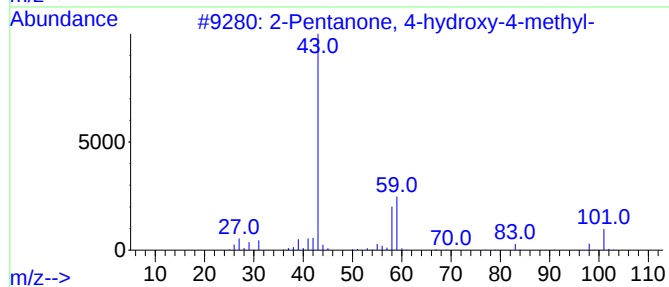
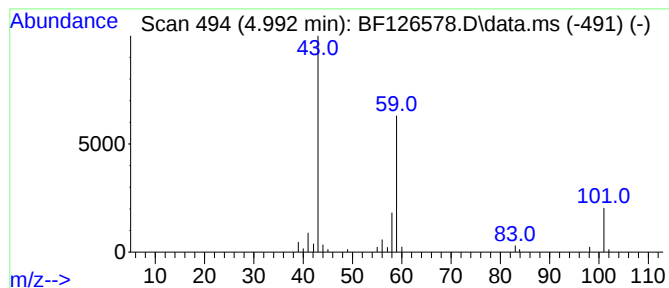
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.992	2.96 ng	78079	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25		
4	3-Hexanol	102	C6H14O	000623-37-0	23		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		



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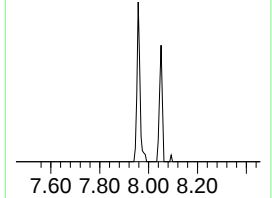
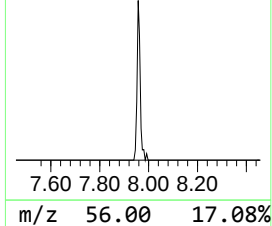
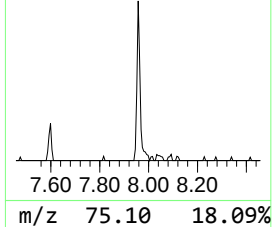
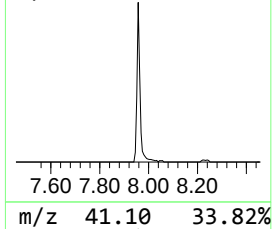
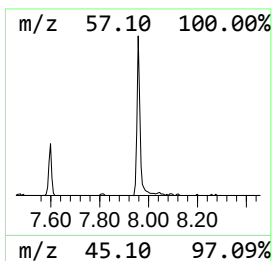
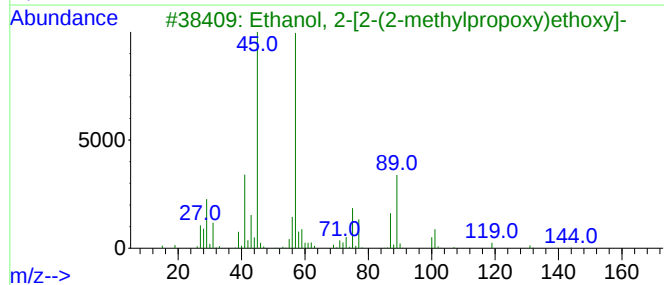
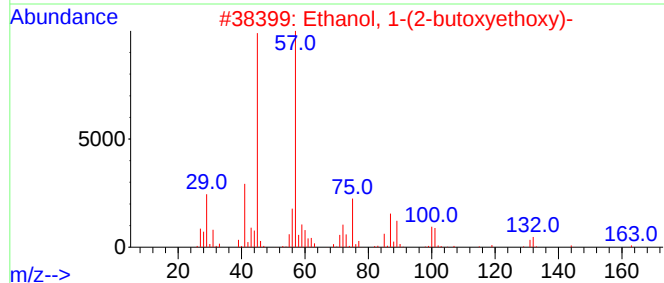
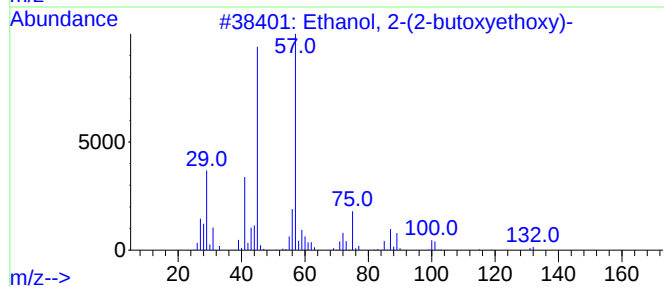
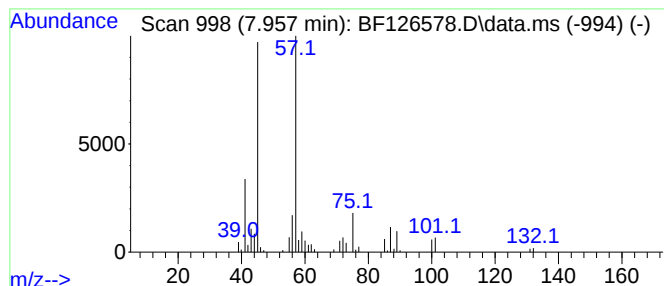
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.957	4.23 ng	149623	Naphthalene-d8	8.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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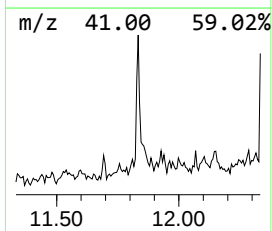
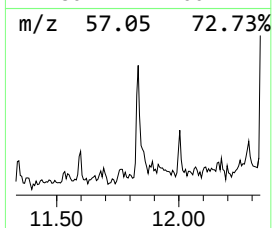
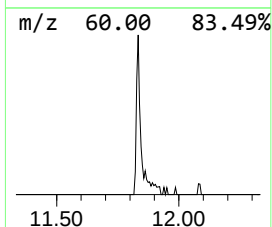
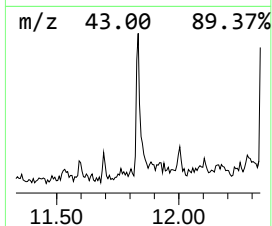
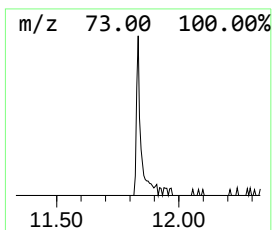
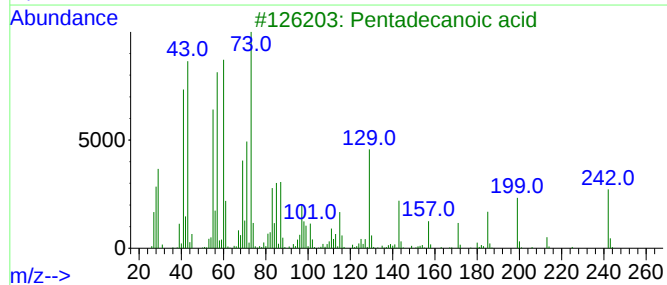
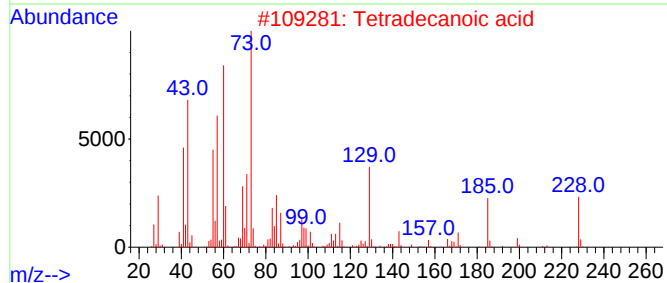
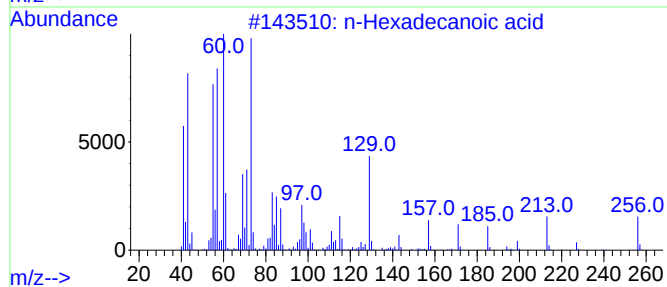
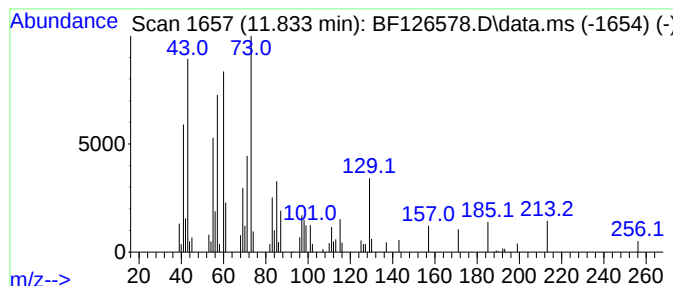
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	3.22 ng	91118	Phenanthrene-d10	11.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



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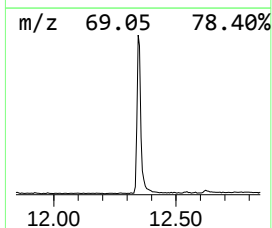
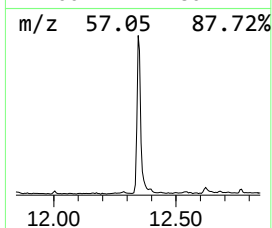
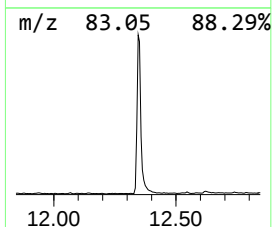
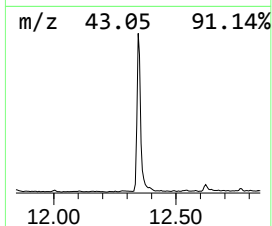
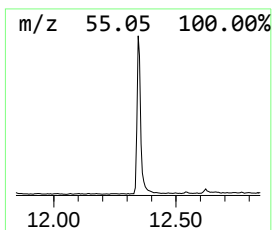
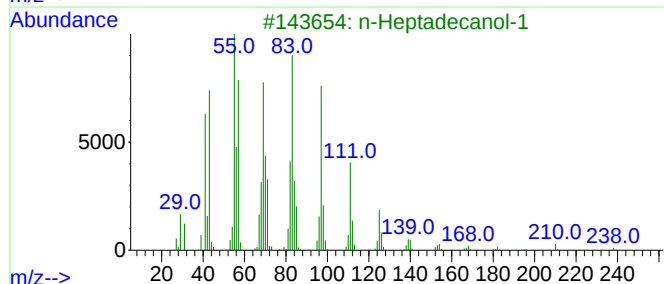
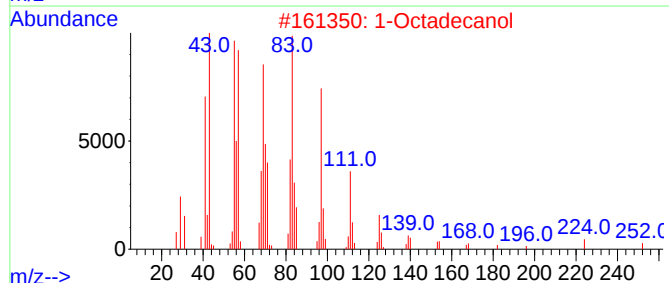
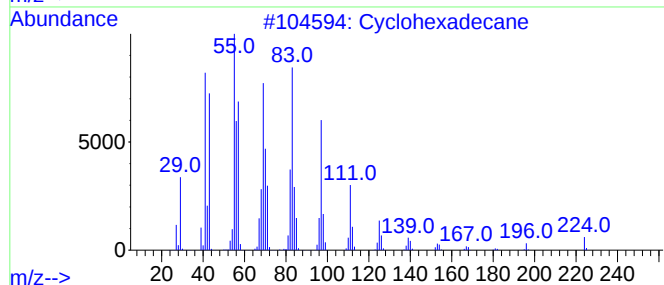
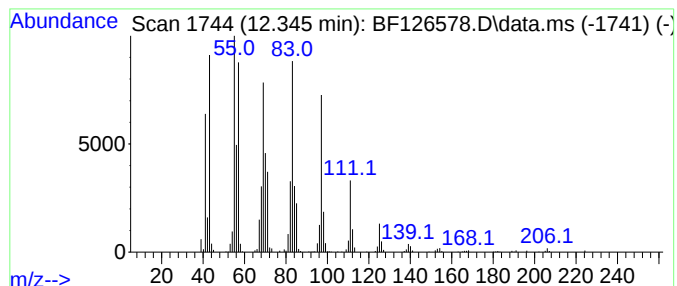
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.345	62.99 ng	1781320	Phenanthrene-d10	11.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			1-Octadecanol	270	C18H38O	000112-92-5	94
3			n-Heptadecanol-1	256	C17H36O	001454-85-9	94
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	94



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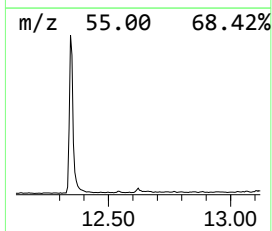
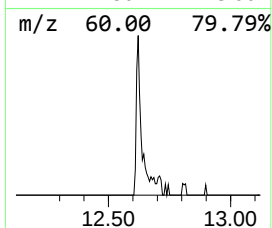
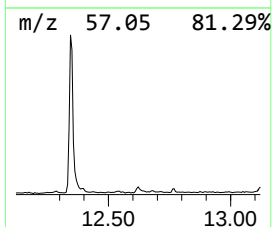
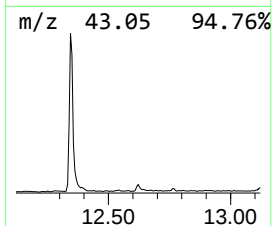
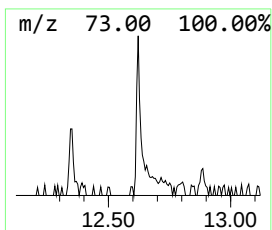
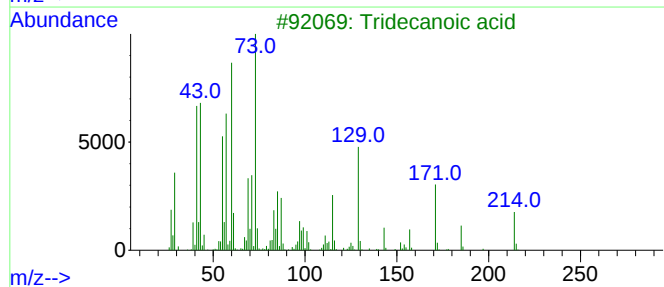
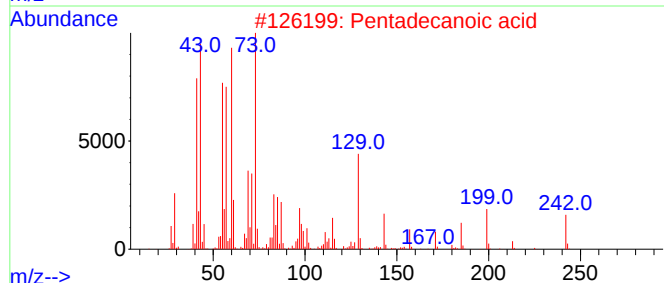
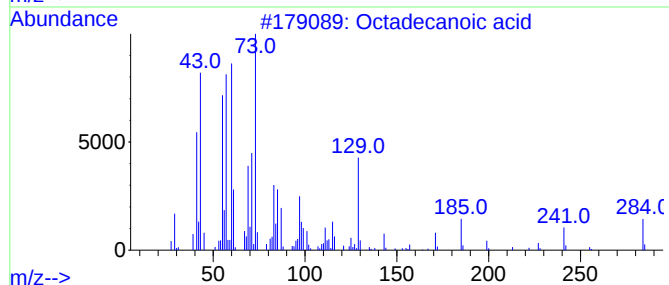
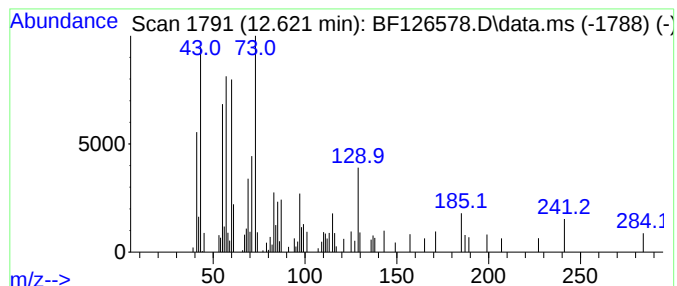
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.621	2.64 ng	78138	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
Data File : BF126578.D
Acq On : 10 Jan 2022 20:35
Operator : JU/CG
Sample : N1080-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

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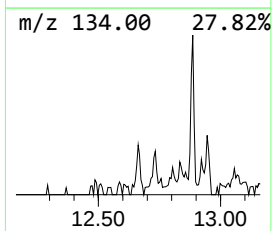
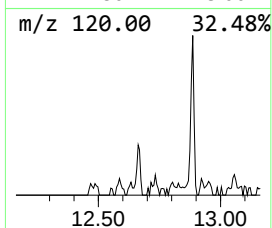
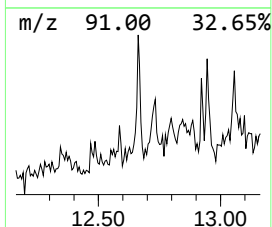
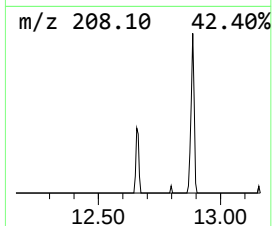
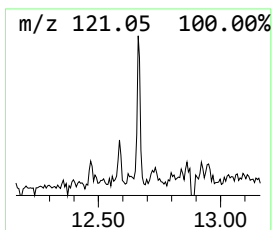
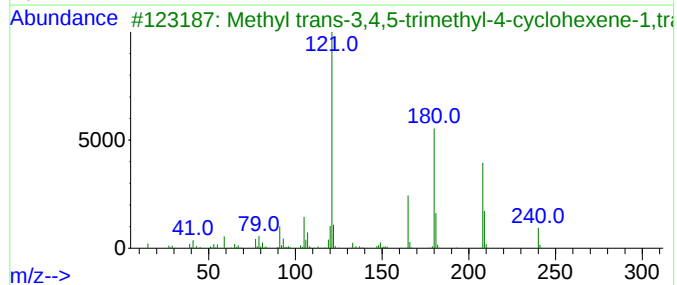
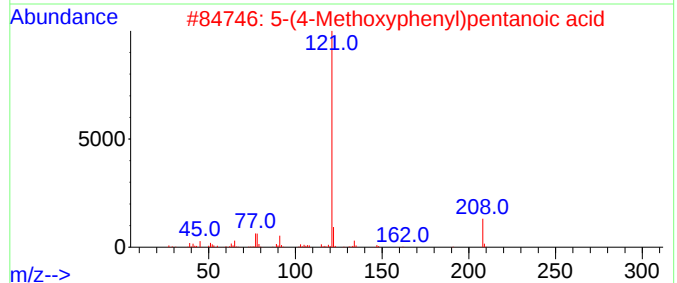
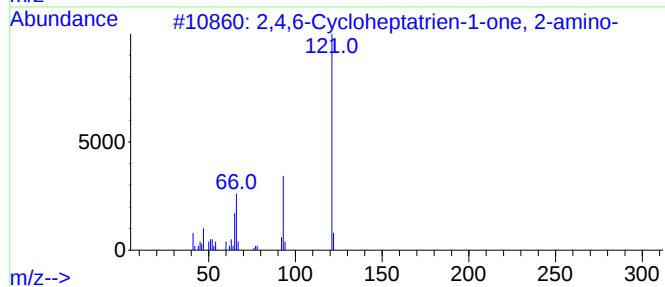
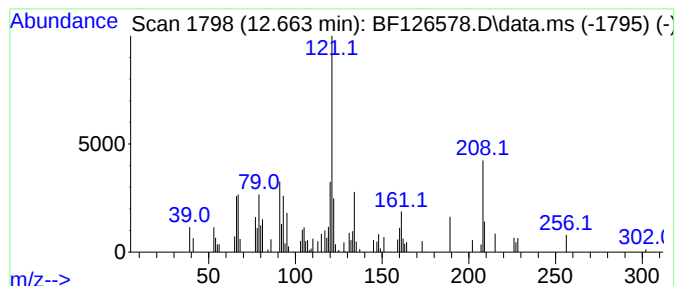
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.663 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	2.14 ng	63261	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4,6-Cycloheptatrien-1-one, 2-a...	121	C7H7NO	006264-93-3	43
2			5-(4-Methoxyphenyl)pentanoic acid	208	C12H16O3	007508-04-5	35
3			Methyl trans-3,4,5-trimethyl-4-c...	240	C13H20O4	1000243-12-5	35
4			4-Methoxybenzyl alcohol, 3-methy...	208	C13H20O2	1000394-77-7	35
5			Benzenamine, 2,3-dimethyl-	121	C8H11N	000087-59-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
Data File : BF126578.D
Acq On : 10 Jan 2022 20:35
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Sample : N1080-02
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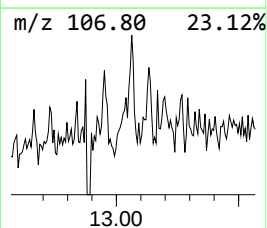
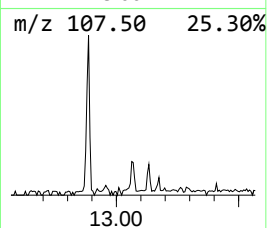
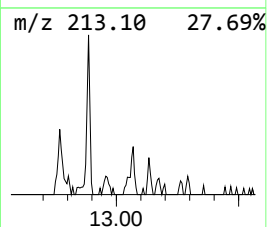
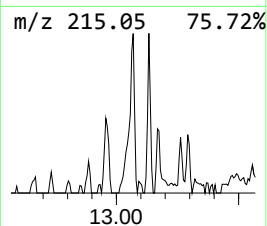
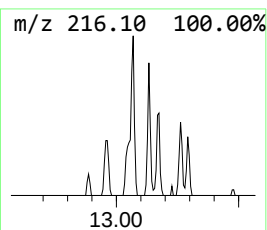
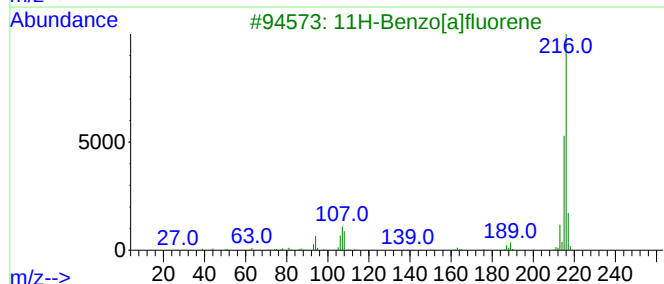
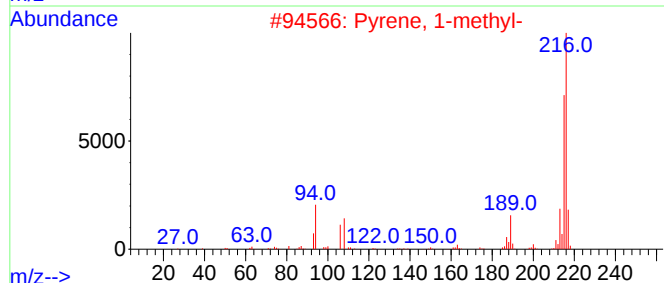
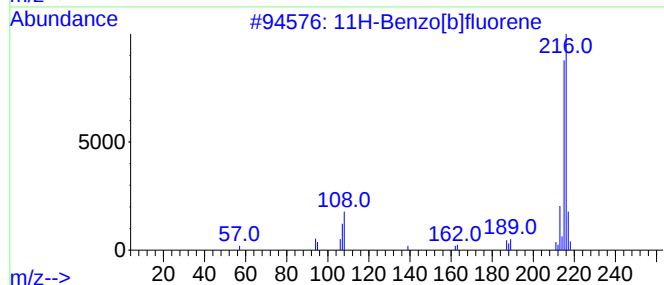
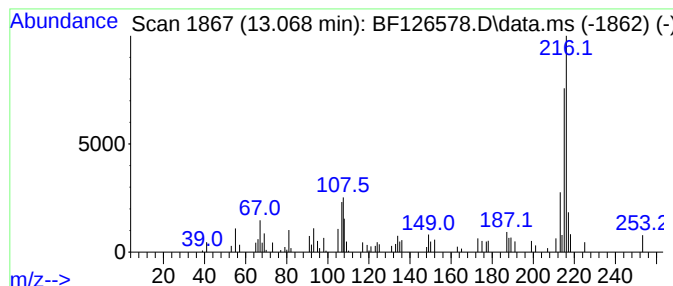
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.069	2.06 ng	60978	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	76
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	76
3			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	72
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
5			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
Data File : BF126578.D
Acq On : 10 Jan 2022 20:35
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Sample : N1080-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

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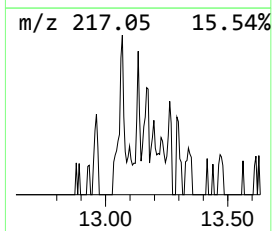
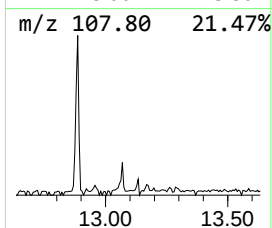
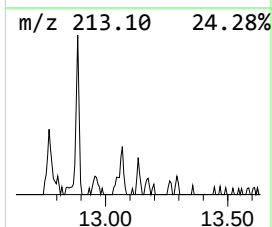
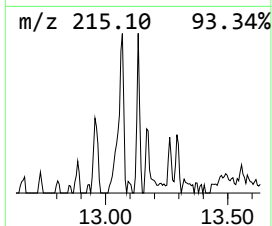
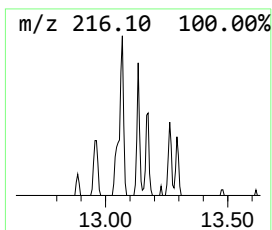
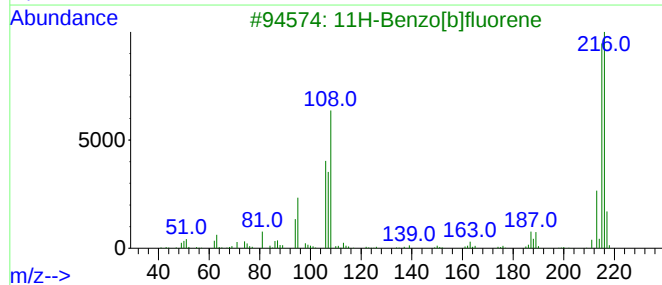
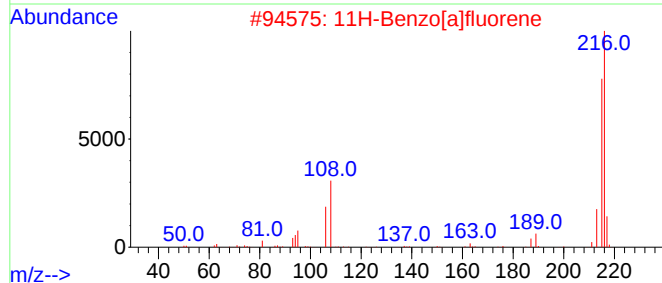
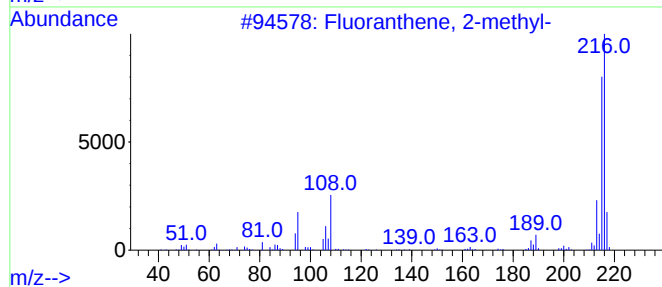
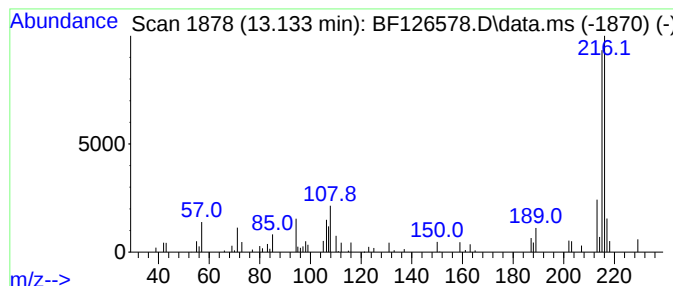
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Fluoranthene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.133	2.10 ng	62072	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
4			Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
5			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
Data File : BF126578.D
Acq On : 10 Jan 2022 20:35
Operator : JU/CG
Sample : N1080-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

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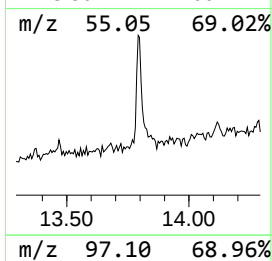
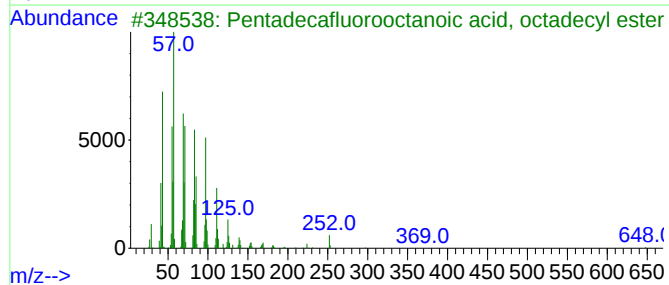
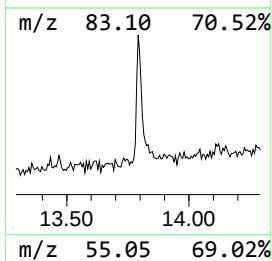
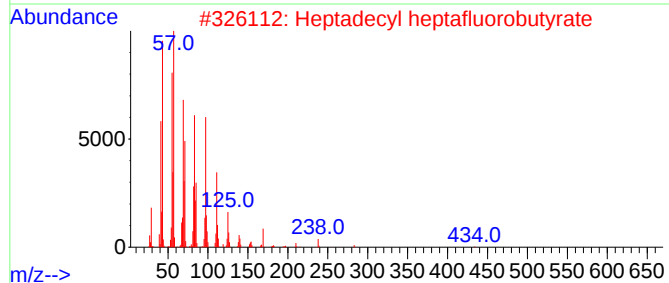
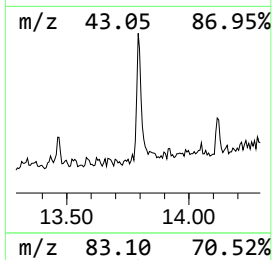
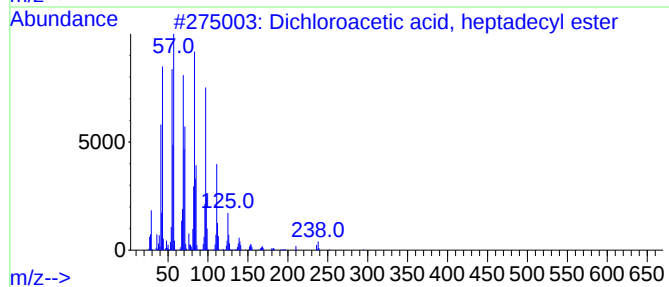
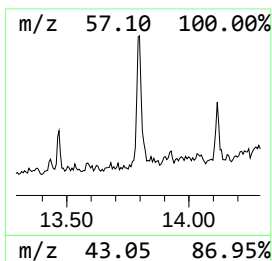
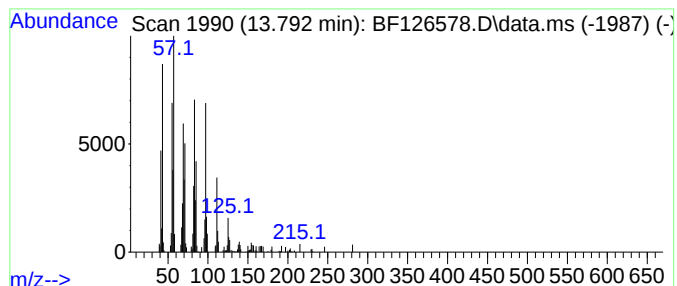
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dichloroacetic acid, heptad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	6.10 ng	180389	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
Data File : BF126578.D
Acq On : 10 Jan 2022 20:35
Operator : JU/CG
Sample : N1080-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

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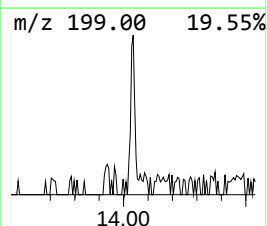
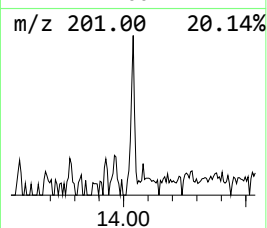
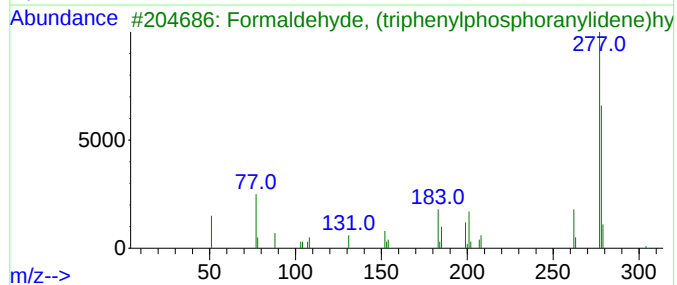
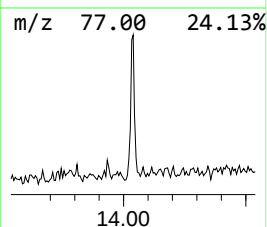
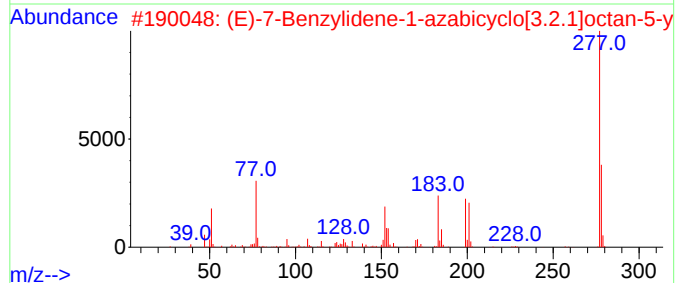
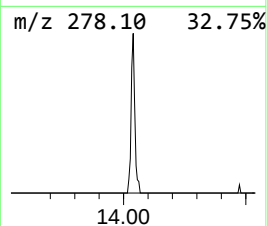
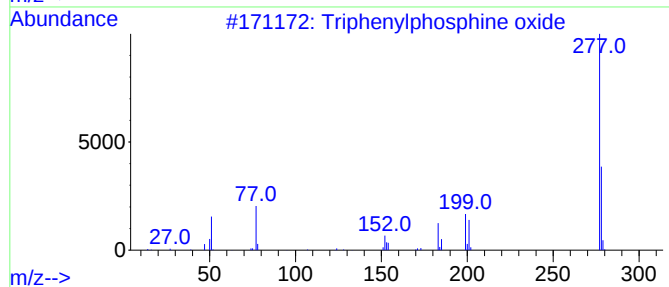
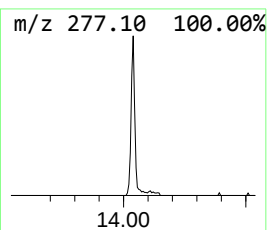
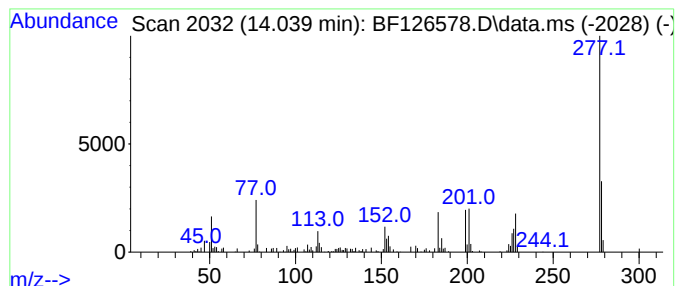
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.039	3.49 ng	103192	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	64
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	40
4			1H-Indole, 3-(2-pyridin-3-yl-thi...]	277	C16H11N3S	1000304-17-8	38
5			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
Data File : BF126578.D
Acq On : 10 Jan 2022 20:35
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ALS Vial : 21 Sample Multiplier: 1

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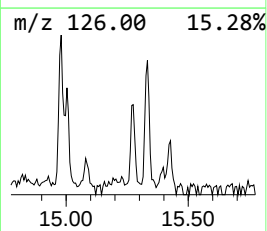
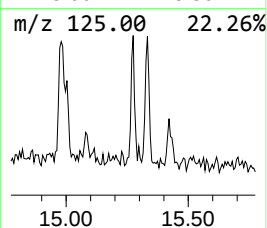
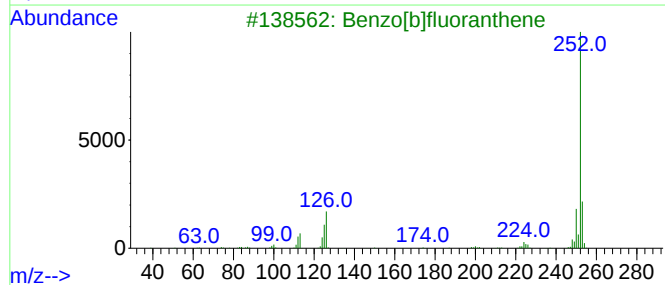
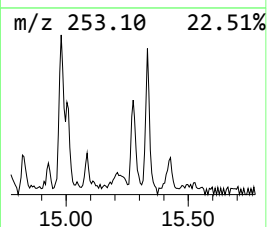
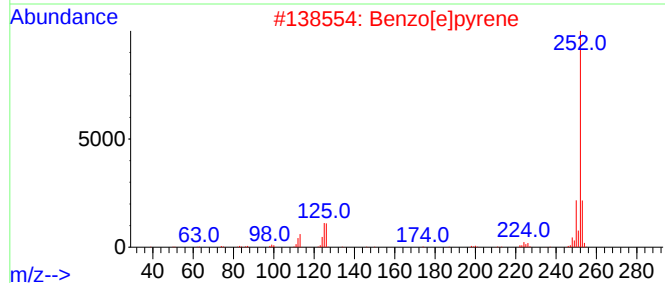
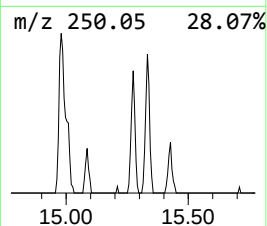
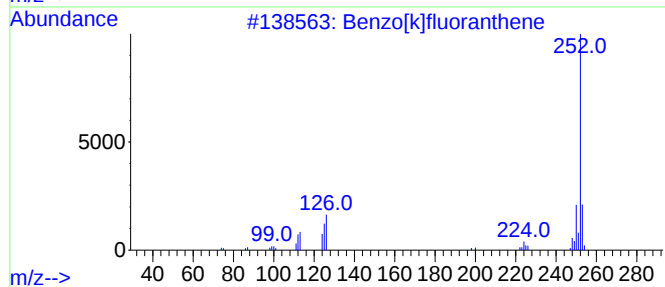
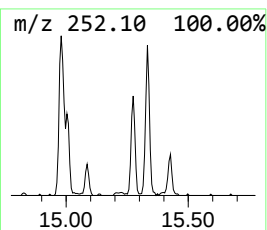
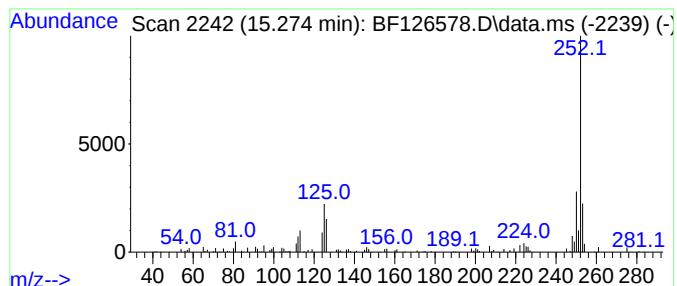
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.274	3.92 ng	91795	Perylene-d12	15.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
2			Benzo[e]pyrene	252	C20H12	000192-97-2	95
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4			Perylene	252	C20H12	000198-55-0	93
5			Benzo[a]pyrene	252	C20H12	000050-32-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
Data File : BF126578.D
Acq On : 10 Jan 2022 20:35
Operator : JU/CG
Sample : N1080-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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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Ethanol, 2-(2-b...	7.957	4.2	ng	149623	2	8.051	707428	20.0
n-Hexadecanoic ...	11.833	3.2	ng	91118	4	11.292	565575	20.0
Cyclohexadecane	12.345	63.0	ng	1781320	4	11.292	565575	20.0
Octadecanoic acid	12.621	2.6	ng	78138	5	13.939	591416	20.0
unknown12.663	12.663	2.1	ng	63261	5	13.939	591416	20.0
11H-Benzo[b]flu...	13.069	2.1	ng	60978	5	13.939	591416	20.0
Fluoranthene, 2...	13.133	2.1	ng	62072	5	13.939	591416	20.0
Dichloroacetic ...	13.792	6.1	ng	180389	5	13.939	591416	20.0
Triphenylphosph...	14.039	3.5	ng	103192	5	13.939	591416	20.0
Benzo[e]pyrene	15.274	3.9	ng	91795	6	15.398	468516	20.0