

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
 Data File : BF125012.D
 Acq On : 9 Aug 2021 21:01
 Operator : JU/CG
 Sample : M3307-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ219-367

Integration Parameters: rteint.p

Integrator: RTE

Smoother: 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-BF080421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125012.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	499	502	505	rBB	5584	6132	3.69%	0.464%
2	5.404	561	564	566	rBV	6237	5831	3.51%	0.441%
3	5.434	566	569	573	rVB	145087	146786	88.40%	11.109%
4	5.651	603	606	610	rBB2	29572	25313	15.24%	1.916%
5	6.340	721	723	726	rBB	3834	2999	1.81%	0.227%
6	6.369	726	728	731	rBB	10297	7812	4.70%	0.591%
7	6.451	738	742	745	rBV	165127	149346	89.94%	11.303%
8	6.645	772	775	778	rBB2	8710	8822	5.31%	0.668%
9	6.816	801	804	807	rBB	45624	35542	21.41%	2.690%
10	7.381	896	900	903	rBB	108441	100951	60.80%	7.640%
11	7.498	917	920	924	rBB	2580	2908	1.75%	0.220%
12	7.645	940	945	951	rBB	10749	13119	7.90%	0.993%
13	8.004	1003	1006	1010	rBB	11872	8673	5.22%	0.656%
14	8.098	1019	1022	1026	rBV	58563	47891	28.84%	3.625%
15	9.175	1201	1205	1208	rBV	205435	166045	100.00%	12.567%
16	9.292	1222	1225	1227	rBB	3230	2650	1.60%	0.201%
17	9.851	1317	1320	1324	rBB	61820	53647	32.31%	4.060%
18	10.645	1451	1455	1458	rBB	117132	95067	57.25%	7.195%
19	11.339	1570	1573	1576	rBV	62736	46190	27.82%	3.496%
20	11.863	1660	1662	1665	rBV	5741	5233	3.15%	0.396%
21	11.898	1665	1668	1672	rVB	96812	77733	46.81%	5.883%
22	12.433	1756	1759	1764	rVB	8774	6007	3.62%	0.455%
23	12.474	1764	1766	1769	rBB	16737	13005	7.83%	0.984%
24	12.522	1770	1774	1776	rBV	2360	2145	1.29%	0.162%
25	12.551	1776	1779	1785	rVB	17707	13935	8.39%	1.055%
26	12.645	1791	1795	1799	rBB2	2368	3013	1.81%	0.228%
27	12.780	1815	1818	1823	rVB	19233	16098	9.69%	1.218%
28	12.922	1838	1842	1845	rBV	137752	111345	67.06%	8.427%
29	13.010	1853	1857	1862	rBV3	5190	6503	3.92%	0.492%
30	13.827	1992	1996	2003	rBB	4260	6709	4.04%	0.508%
31	13.974	2014	2021	2024	rBV3	36526	44939	27.06%	3.401%
32	14.004	2024	2026	2028	rVB	8519	6452	3.89%	0.488%
33	15.010	2193	2197	2199	rBV	11582	13201	7.95%	0.999%
34	15.027	2199	2200	2204	rVV	4762	5309	3.20%	0.402%
35	15.068	2204	2207	2210	rVB	2465	2663	1.60%	0.202%
36	15.304	2245	2247	2252	rBB	6140	6396	3.85%	0.484%

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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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.368	2255	2258	2265	rBB	10004	9795	5.90%	0.741%
38	15.433	2265	2269	2273	rBV	30571	34461	20.75%	2.608%
39	16.292	2410	2415	2416	rBV2	1626	2393	1.44%	0.181%
40	16.880	2510	2515	2519	rBB3	3642	4656	2.80%	0.352%
41	17.315	2585	2589	2594	rBB	2747	3595	2.17%	0.272%

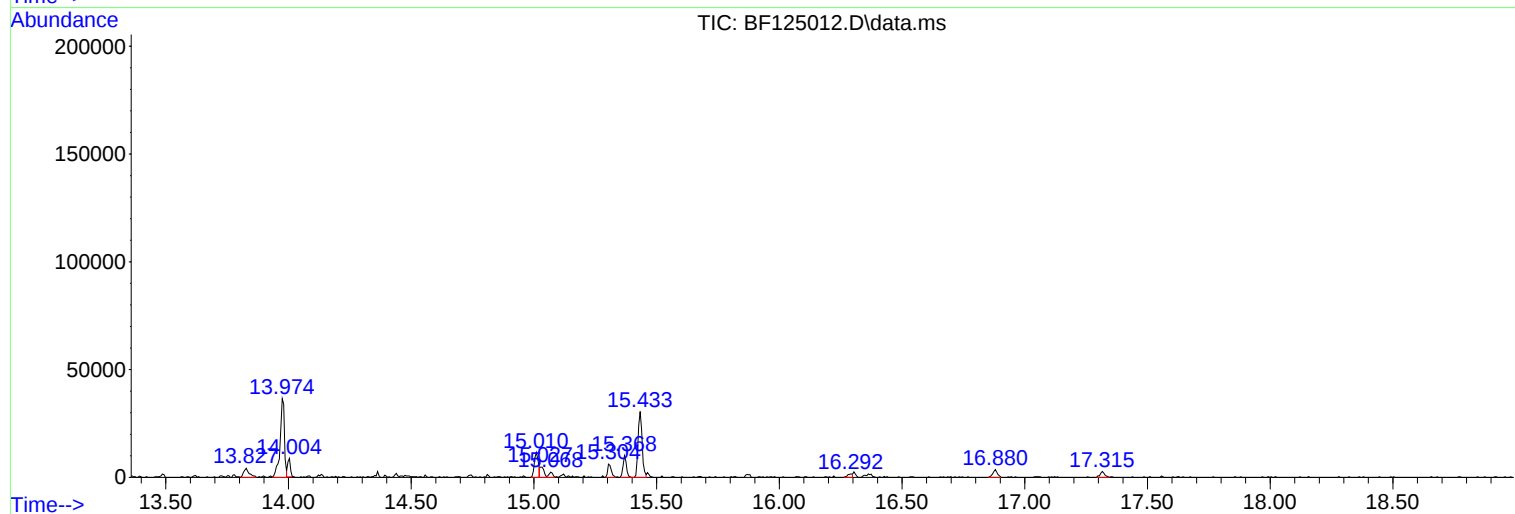
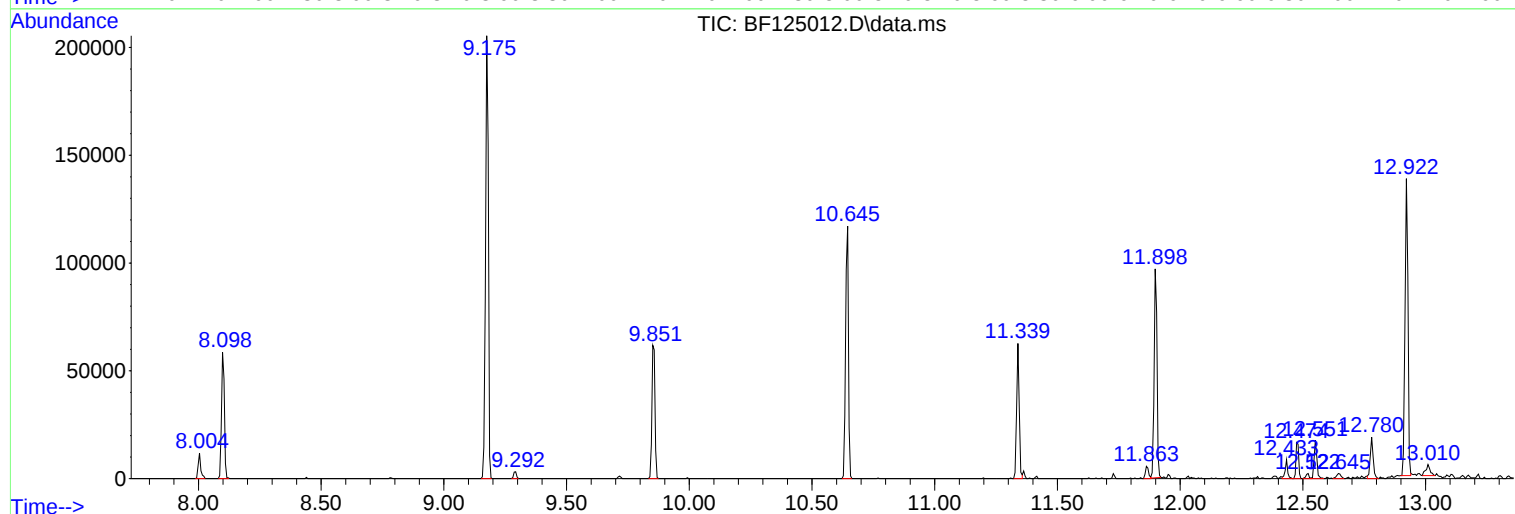
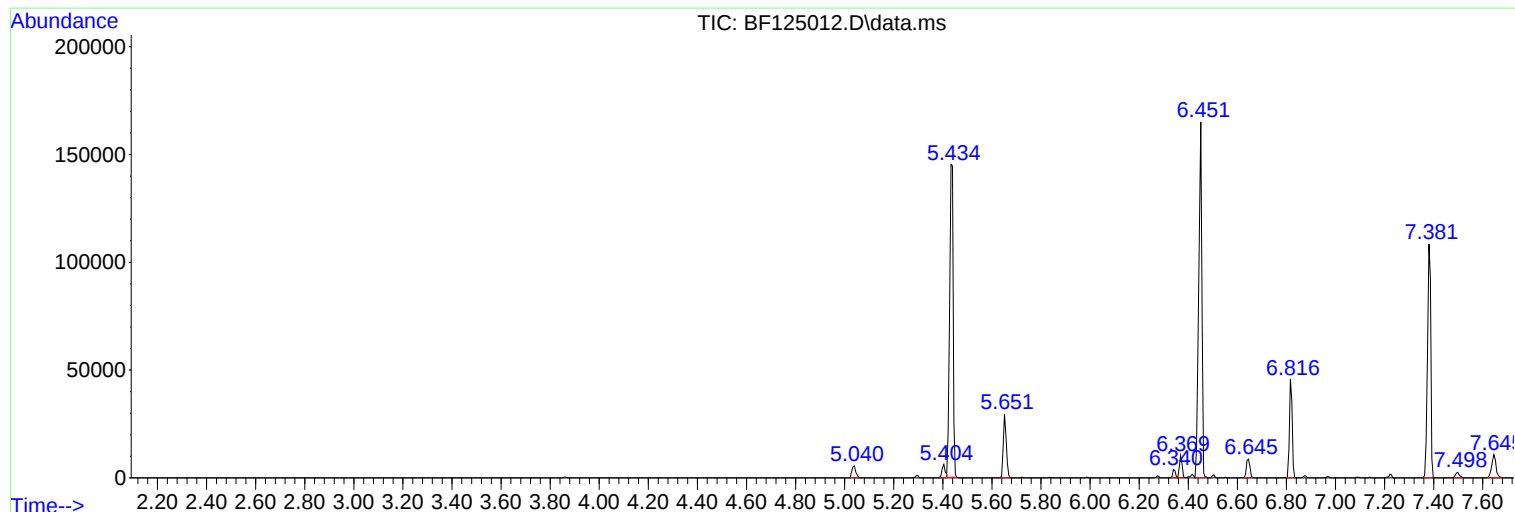
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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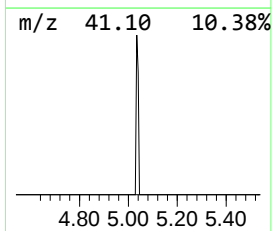
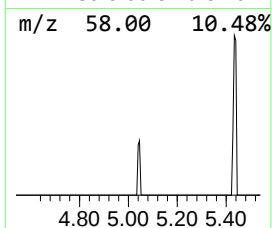
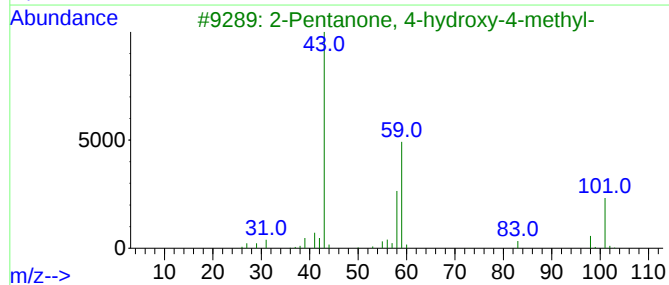
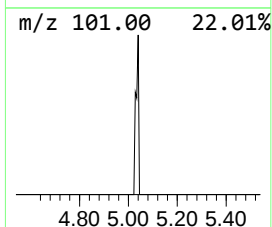
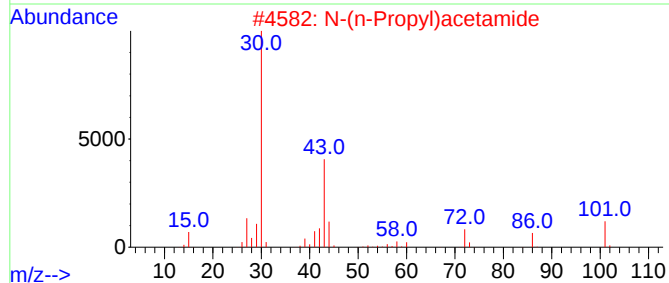
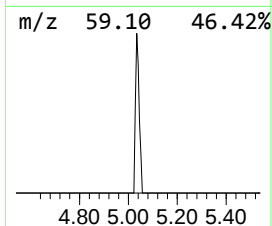
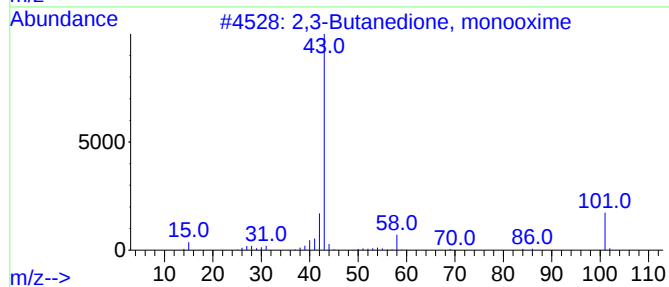
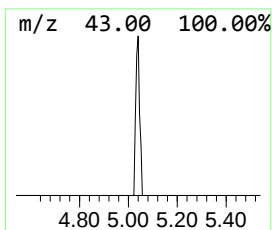
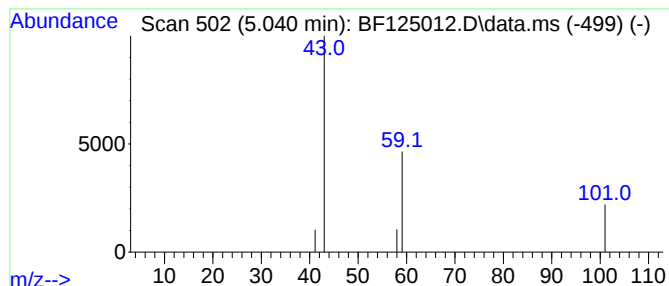
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.040 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	3.45 ng	6132	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	7	
2	N-(n-Propyl)acetamide		101	C5H11NO	005331-48-6	4	
3	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	4	
4	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	4	
5	Propylamine		59	C3H9N	000107-10-8	3	



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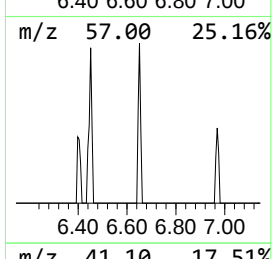
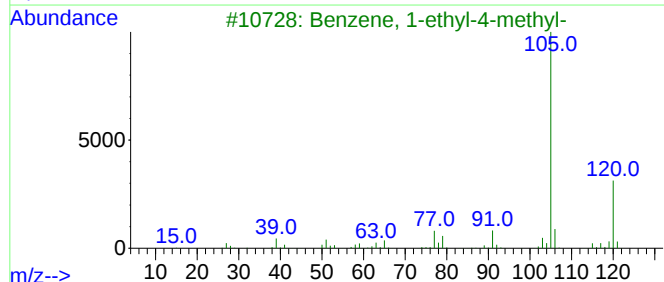
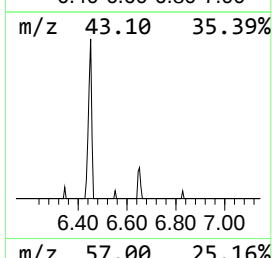
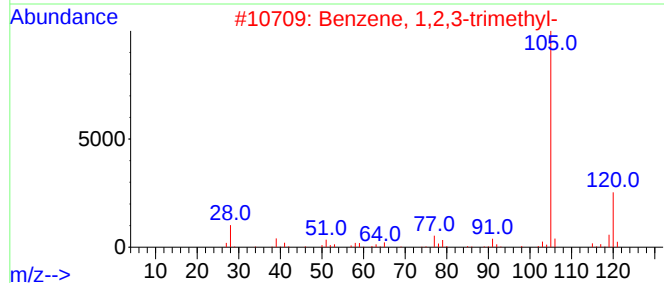
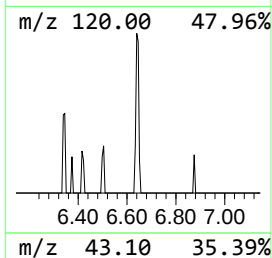
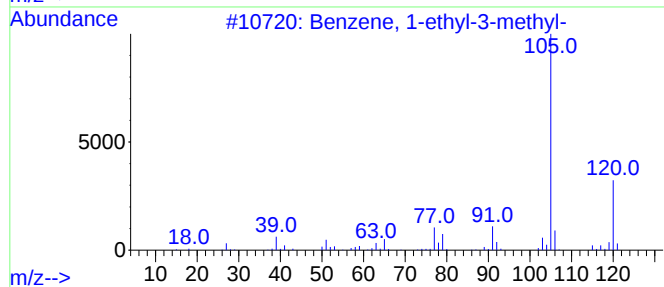
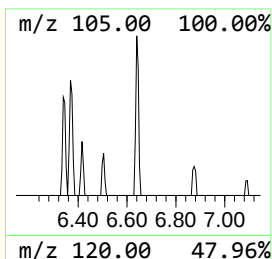
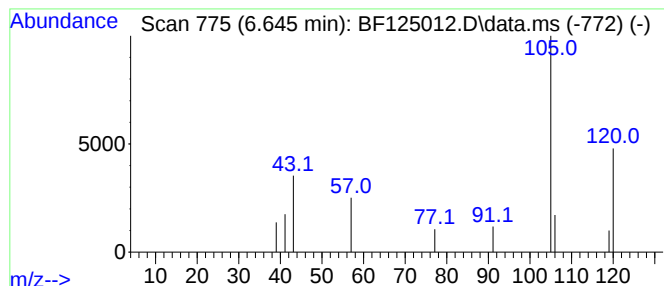
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Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.645	4.96 ng	8822	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	74
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	9
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	9
4			Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	7
5			2,4-Heptadien-6-ynal, (E,E)-	106	C7H6O	007200-04-6	7



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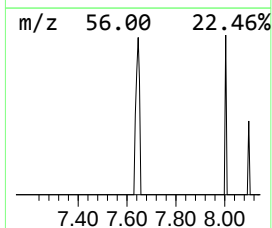
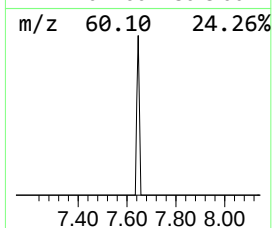
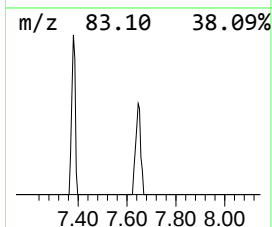
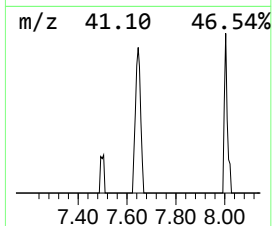
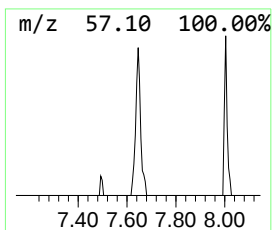
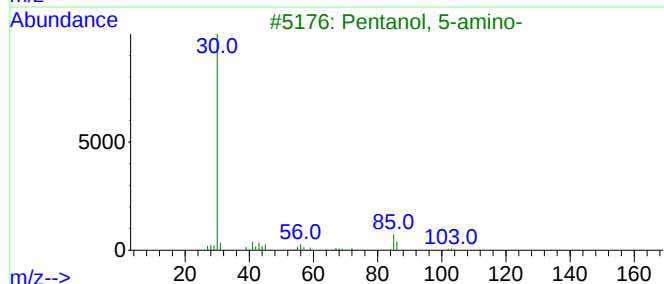
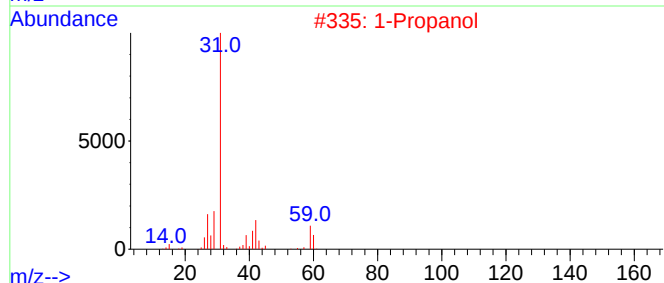
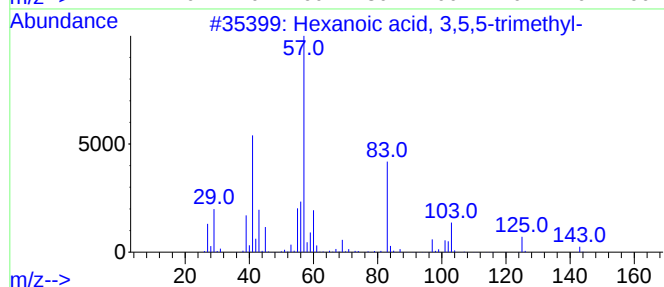
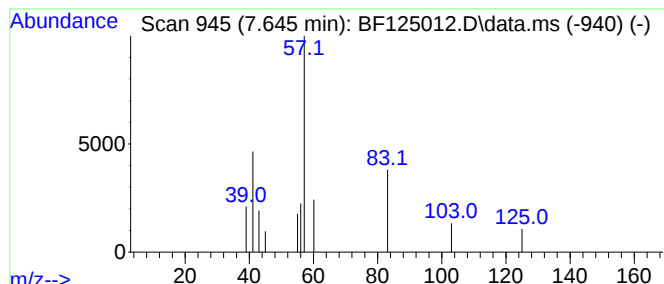
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexanoic acid, 3,5,5-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.645	5.48 ng	13119	Naphthalene-d8	8.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	83
2			1-Propanol	60	C3H8O	000071-23-8	5
3			Pentanol, 5-amino-	103	C5H13NO	002508-29-4	4
4			Propanoic acid, 3-amino-2-methyl-	103	C4H9NO2	000144-90-1	4
5			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	4



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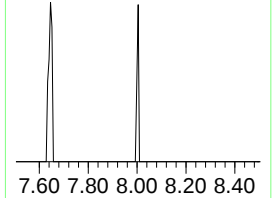
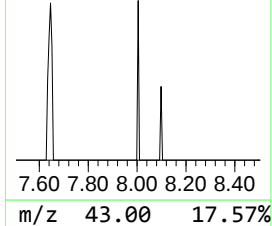
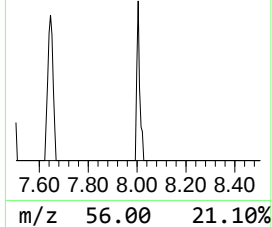
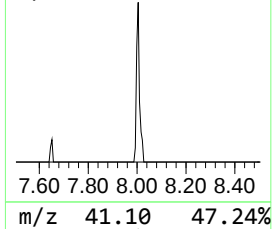
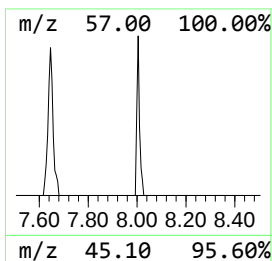
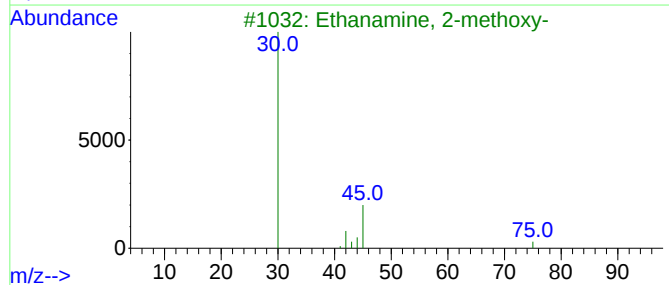
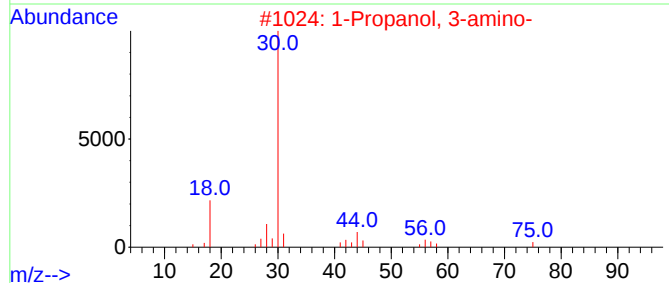
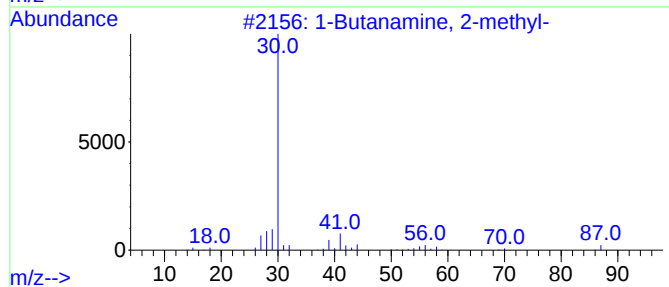
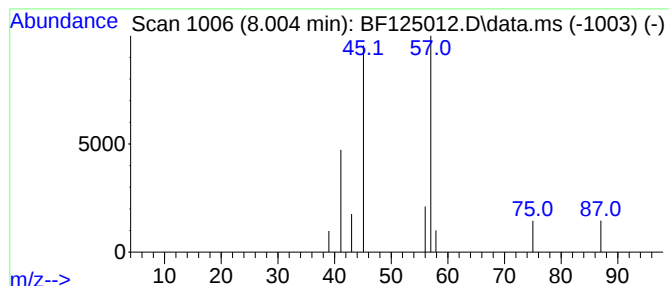
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown8.004 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	3.62 ng	8673	Naphthalene-d8	8.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	5
2			1-Propanol, 3-amino-	75	C3H9NO	000156-87-6	5
3			Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	4
4			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	4
5			Sulfone, 2-hydroxypropyl t-butyl	180	C7H16O3S	154619-05-3	4



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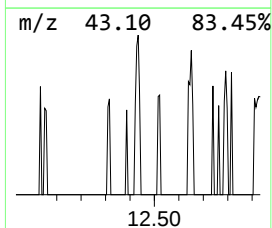
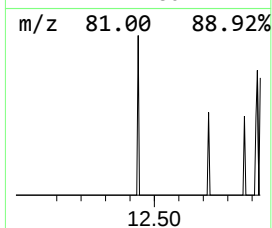
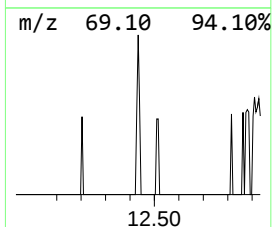
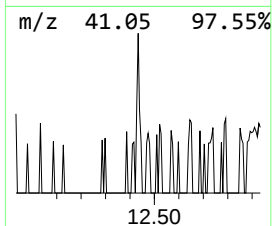
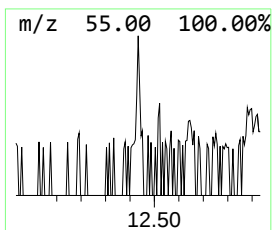
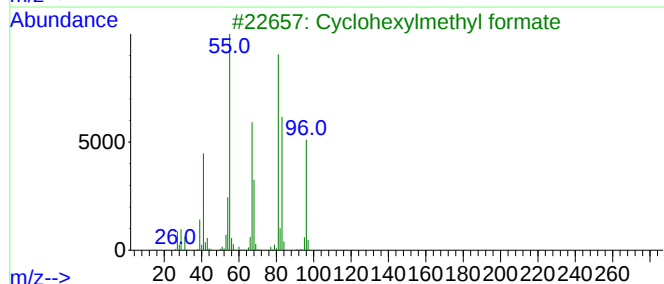
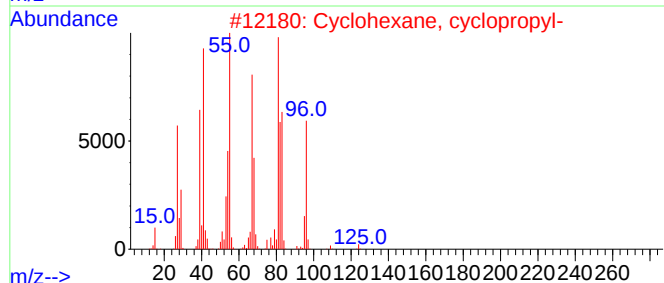
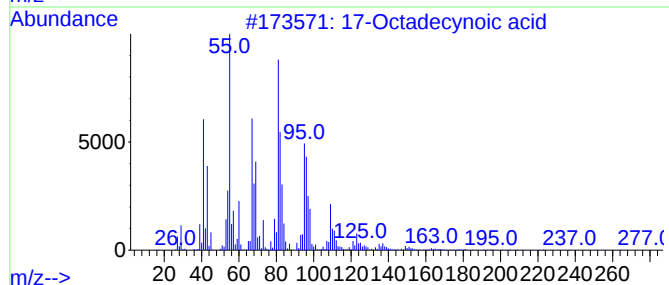
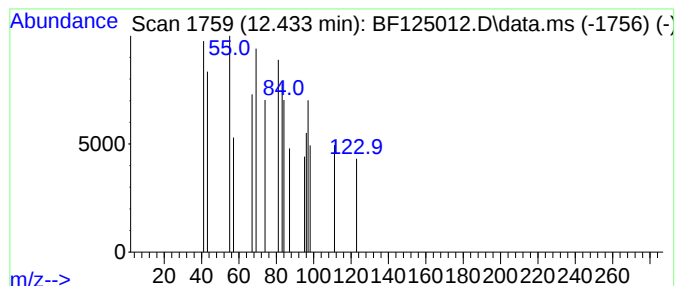
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.433 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	2.60 ng	6007	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Octadecynoic acid	280	C18H32O2	034450-18-5	35
2			Cyclohexane, cyclopropyl-	124	C9H16	032669-86-6	35
3			Cyclohexylmethyl formate	142	C8H14O2	002888-49-5	35
4			1-Octadecyne	250	C18H34	000629-89-0	27
5			2-Hexenal	98	C6H10O	000505-57-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125012.D
Acq On : 9 Aug 2021 21:01
Operator : JU/CG
Sample : M3307-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ219-367

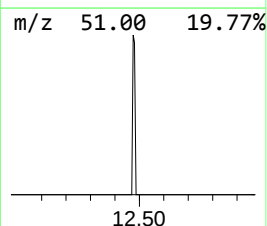
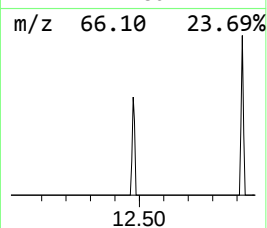
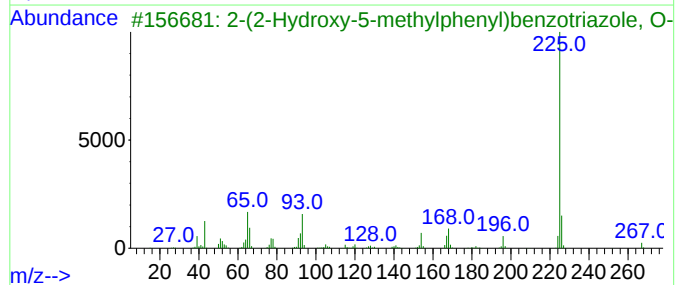
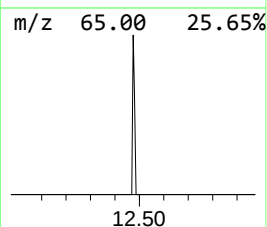
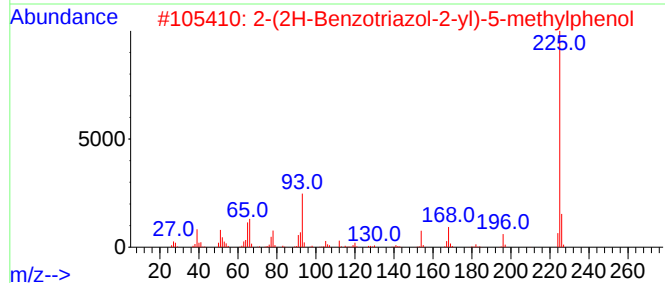
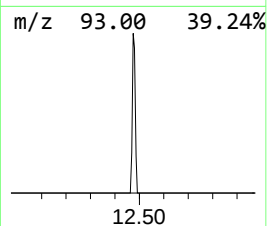
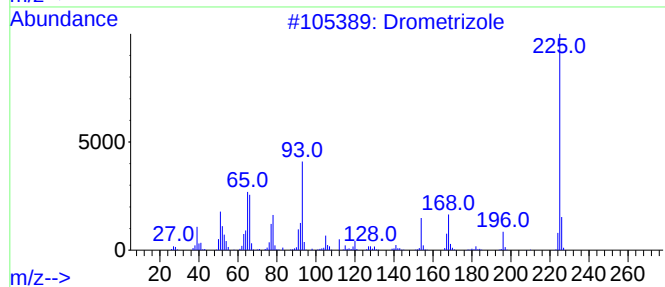
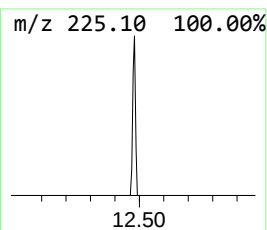
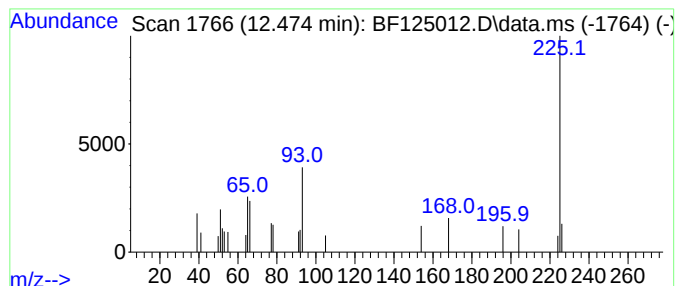
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Drometrizole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.475	5.63 ng	13005	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Drometrizole	225	C13H11N3O	002440-22-4	96
2			2-(2H-Benzotriazol-2-yl)-5-methy...	225	C13H11N3O	004998-48-5	91
3			2-(2-Hydroxy-5-methylphenyl)benz...	267	C15H13N3O2	1000384-15-2	47
4			4,5-Diamino-2-phenyl(2H)benzotri...	225	C12H11N5	166766-26-3	35
5			Phenazine, 1-amino-3-methoxy-	225	C13H11N3O	018450-06-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125012.D
Acq On : 9 Aug 2021 21:01
Operator : JU/CG
Sample : M3307-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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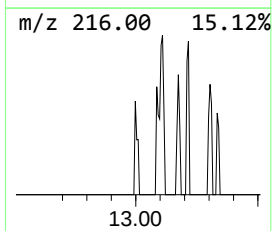
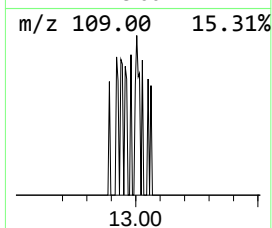
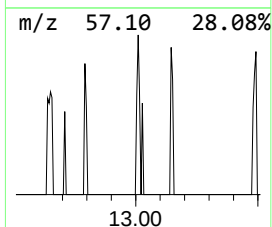
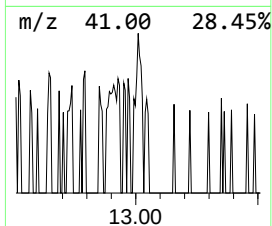
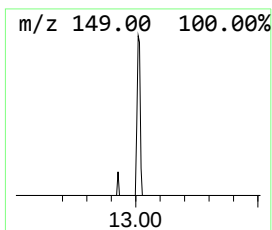
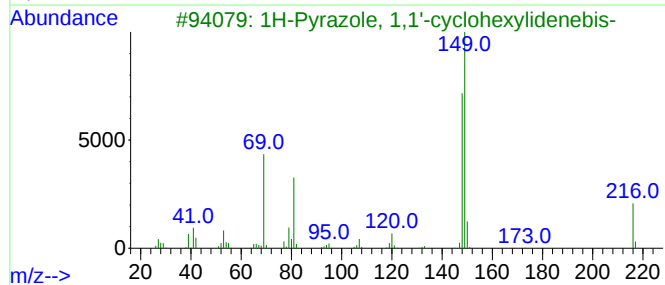
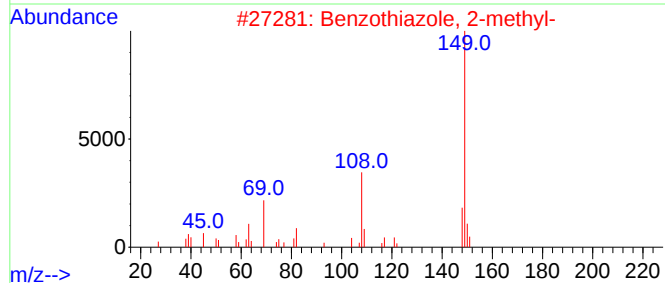
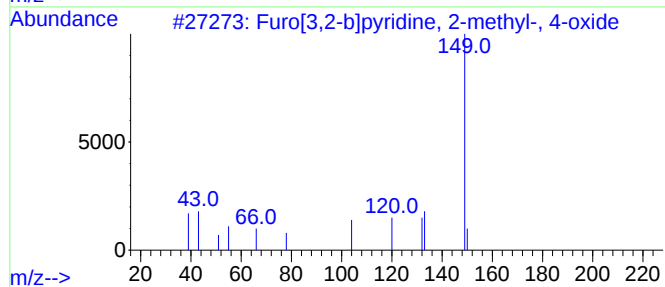
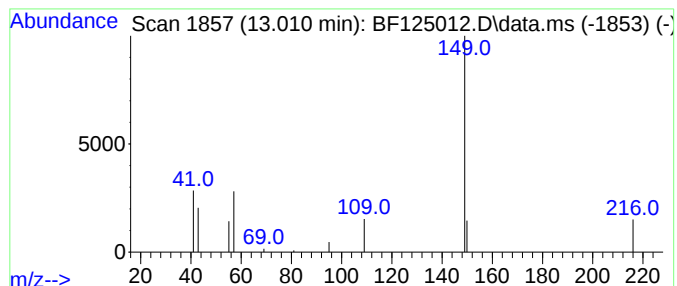
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.010 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.010	2.89 ng	6503	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furo[3,2-b]pyridine, 2-methyl-, ...	149	C8H7NO2	069022-83-9	9
2			Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	7
3			1H-Pyrazole, 1,1'-cyclohexyliden...	216	C12H16N4	028791-88-0	5
4			Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
5			Formamide, N-ethyl-N-phenyl-	149	C9H11NO	005461-49-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125012.D
Acq On : 9 Aug 2021 21:01
Operator : JU/CG
Sample : M3307-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ219-367

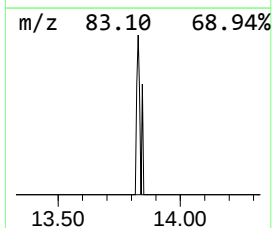
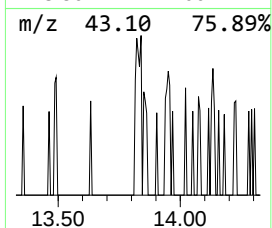
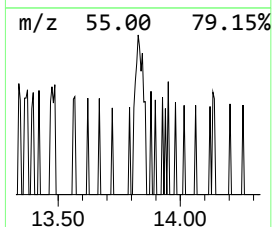
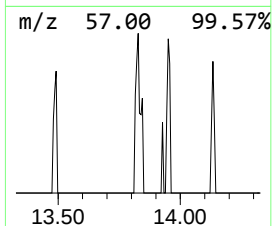
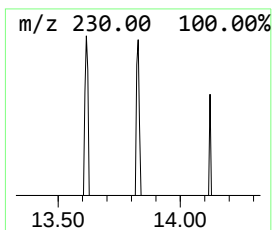
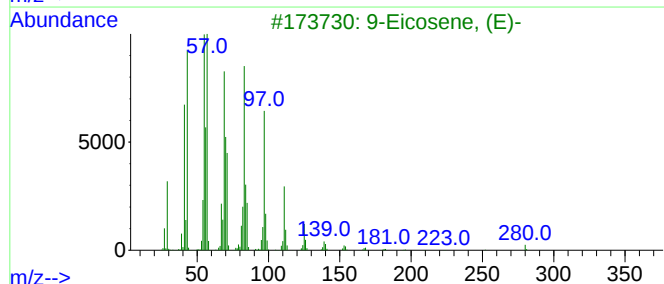
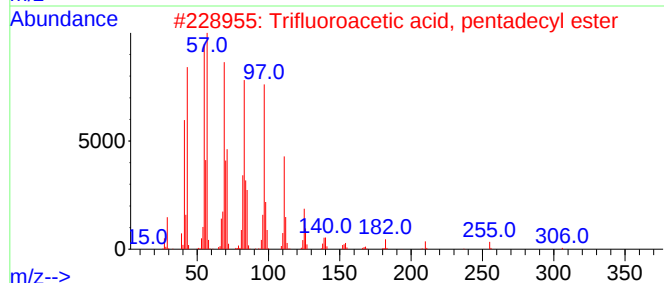
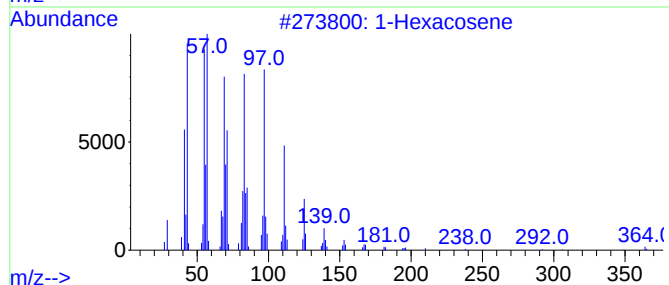
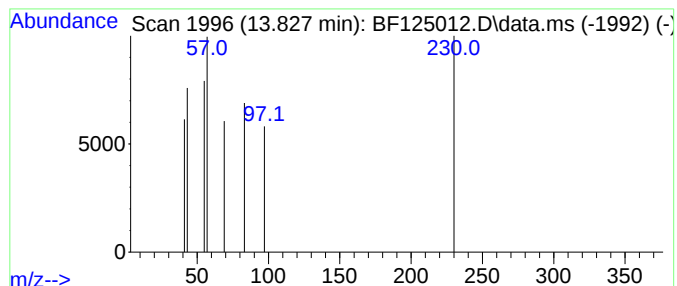
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.827 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	2.99 ng	6709	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene		364	C26H52		018835-33-1	47
2	Trifluoroacetic acid, pentadecyl...		324	C17H31F3O2		959010-23-2	47
3	9-Eicosene, (E)-		280	C20H40		074685-29-3	47
4	Pentafluoropropionic acid, tetra...		360	C17H29F5O2		006222-06-6	47
5	1-Heptadecene		238	C17H34		006765-39-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125012.D
Acq On : 9 Aug 2021 21:01
Operator : JU/CG
Sample : M3307-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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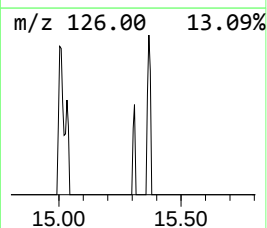
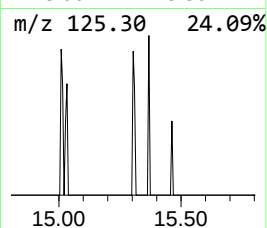
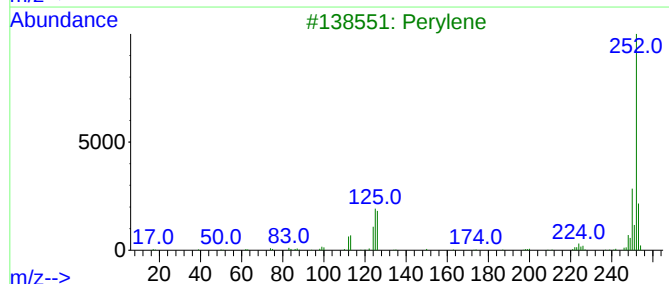
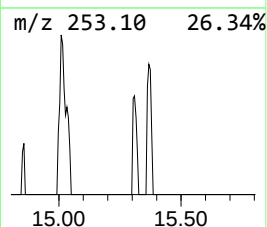
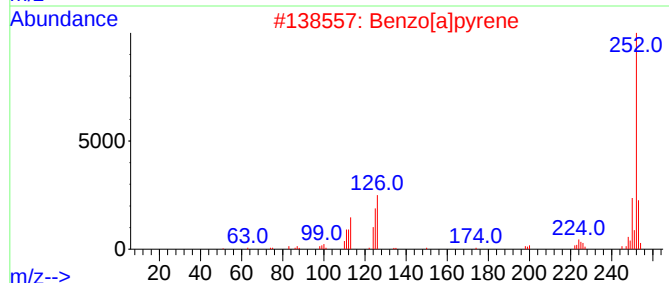
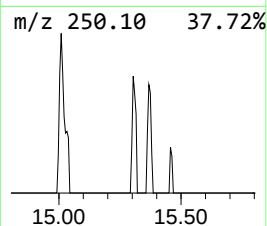
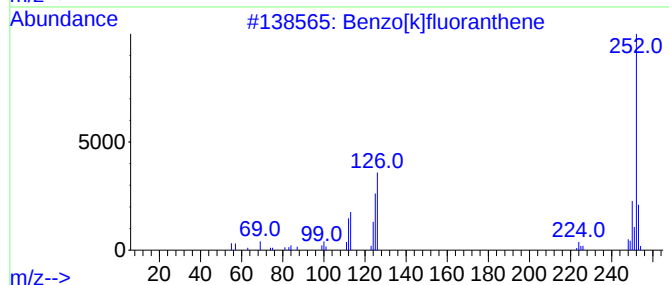
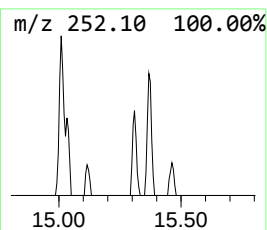
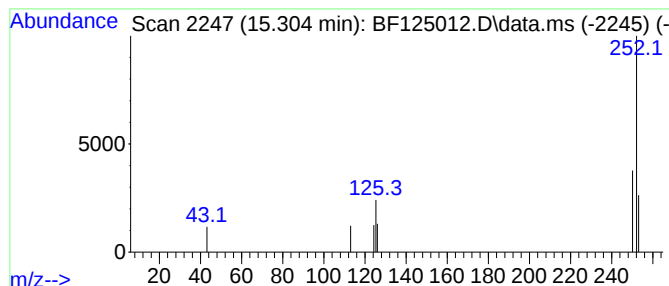
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.304	3.71 ng	6396	Perylene-d12	15.433

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[k]fluoranthene	252	C20H12	000207-08-9	64
2		Benzo[a]pyrene	252	C20H12	000050-32-8	64
3		Perylene	252	C20H12	000198-55-0	50
4		Benzo[e]pyrene	252	C20H12	000192-97-2	50
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125012.D
Acq On : 9 Aug 2021 21:01
Operator : JU/CG
Sample : M3307-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ219-367

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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Benzene, 1-ethy...	6.645	5.0	ng	8822	1	6.816	35542	20.0
Hexanoic acid, ...	7.645	5.5	ng	13119	2	8.098	47891	20.0
unknown8.004	8.004	3.6	ng	8673	2	8.098	47891	20.0
unknown12.433	12.433	2.6	ng	6007	4	11.339	46190	20.0
Drometrizole	12.475	5.6	ng	13005	4	11.339	46190	20.0
unknown13.010	13.010	2.9	ng	6503	5	13.980	44939	20.0
unknown13.827	13.827	3.0	ng	6709	5	13.980	44939	20.0
Perylene	15.304	3.7	ng	6396	6	15.433	34461	20.0