

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022323\
 Data File : BF132530.D
 Acq On : 23 Feb 2023 20:24
 Operator : CG\JU
 Sample : 01659-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 QAQC-COMP-2

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132530.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.248	404	410	418	rVB	1445253	1842722	47.38%	5.573%
2	5.637	472	476	480	rBV	3506379	3428610	88.15%	10.370%
3	5.854	509	513	520	rBV	62961	71332	1.83%	0.216%
4	6.637	641	646	649	rBV	3462883	3424044	88.04%	10.356%
5	6.842	676	681	685	rBV2	63398	93909	2.41%	0.284%
6	7.007	705	709	712	rBV	1213043	932265	23.97%	2.820%
7	7.272	749	754	760	rBV	71540	91153	2.34%	0.276%
8	7.572	800	805	808	rBV	2630072	2274458	58.48%	6.879%
9	7.866	852	855	858	rBV	109884	104976	2.70%	0.317%
10	8.089	888	893	901	rVB	44610	64120	1.65%	0.194%
11	8.295	924	928	930	rBV	1335427	1189131	30.57%	3.596%
12	8.313	930	931	934	rVB	109890	62272	1.60%	0.188%
13	8.507	960	964	967	rBV	72984	68376	1.76%	0.207%
14	8.566	970	974	977	rBV	98184	89633	2.30%	0.271%
15	9.001	1045	1048	1052	rBV2	98036	87699	2.25%	0.265%
16	9.372	1106	1111	1114	rVB	4238884	3889408	100.00%	11.763%
17	9.436	1119	1122	1125	rVB2	53740	43983	1.13%	0.133%
18	9.495	1130	1132	1141	rBV	254842	267702	6.88%	0.810%
19	9.913	1200	1203	1206	rBV	48112	44338	1.14%	0.134%
20	9.995	1214	1217	1219	rBV	83389	79617	2.05%	0.241%
21	10.019	1219	1221	1224	rVV2	53768	64617	1.66%	0.195%
22	10.054	1224	1227	1230	rVV	1619651	1294174	33.27%	3.914%
23	10.083	1230	1232	1236	rVB	172687	148202	3.81%	0.448%
24	10.260	1259	1262	1265	rVB	69995	63597	1.64%	0.192%
25	10.472	1295	1298	1301	rVB2	43611	46272	1.19%	0.140%
26	10.601	1317	1320	1325	rBV	92605	88492	2.28%	0.268%
27	10.766	1345	1348	1351	rVB2	143922	122060	3.14%	0.369%
28	10.848	1358	1362	1365	rBV	2472135	2160318	55.54%	6.534%
29	10.960	1376	1381	1388	rVB3	81713	137615	3.54%	0.416%
30	11.354	1445	1448	1452	rVB2	41661	46681	1.20%	0.141%
31	11.395	1452	1455	1458	rVV3	79658	79389	2.04%	0.240%
32	11.442	1462	1463	1468	rVB	46154	44956	1.16%	0.136%
33	11.548	1477	1481	1483	rBV	1272469	1092929	28.10%	3.306%
34	11.572	1483	1485	1489	rVV	668030	551103	14.17%	1.667%
35	11.624	1489	1494	1496	rVV	157880	152661	3.93%	0.462%
36	11.648	1496	1498	1505	rVB4	35916	53155	1.37%	0.161%

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37	11.777	1517	1520	1525	rVB	79546	69498	1.79%	0.210%
38	12.060	1564	1568	1570	rBV2	310050	299345	7.70%	0.905%
39	12.077	1570	1571	1575	rVB	97202	79088	2.03%	0.239%
40	12.166	1583	1586	1589	rBV	106436	117911	3.03%	0.357%
41	12.771	1685	1689	1692	rBV	742051	664160	17.08%	2.009%
42	12.848	1700	1702	1707	rVB4	50080	56608	1.46%	0.171%
43	13.001	1725	1728	1734	rVB	693398	621656	15.98%	1.880%
44	13.136	1745	1751	1755	rBV	2836425	2647022	68.06%	8.006%
45	13.224	1761	1766	1769	rBV2	36031	62543	1.61%	0.189%
46	13.330	1781	1784	1786	rVB	74397	60207	1.55%	0.182%
47	13.560	1820	1823	1826	rBV2	41020	49108	1.26%	0.149%
48	13.836	1868	1870	1875	rVB	54934	57610	1.48%	0.174%
49	14.030	1900	1903	1913	rVB4	238189	412330	10.60%	1.247%
50	14.166	1924	1926	1928	rBV2	66586	60667	1.56%	0.183%
51	14.207	1928	1933	1935	rVV2	949706	1161320	29.86%	3.512%
52	14.230	1935	1937	1943	rVB	317980	274414	7.06%	0.830%
53	14.660	2007	2010	2012	rBV2	54373	62564	1.61%	0.189%
54	15.295	2114	2118	2121	rBV	256373	396207	10.19%	1.198%
55	15.618	2170	2173	2180	rVB	142820	205757	5.29%	0.622%
56	15.689	2181	2185	2191	rVB	213090	284102	7.30%	0.859%
57	15.760	2192	2197	2201	rBV	674765	865113	22.24%	2.617%
58	15.989	2232	2236	2241	rBV2	74609	106380	2.74%	0.322%
59	17.354	2464	2468	2475	rVB3	76397	154140	3.96%	0.466%

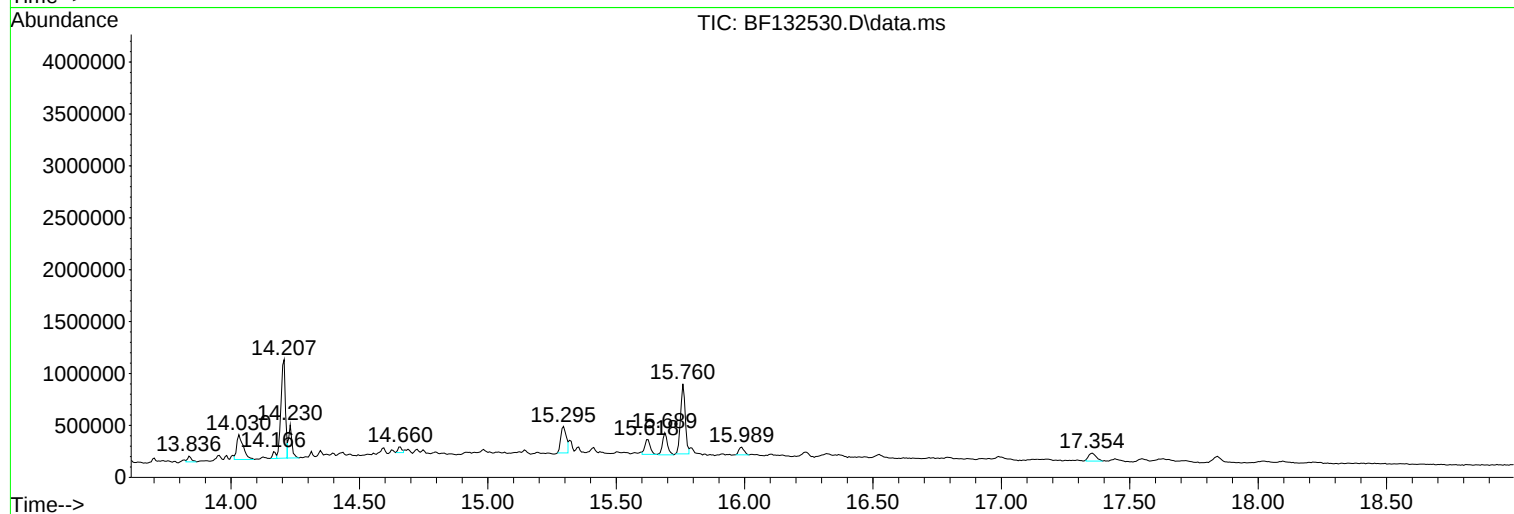
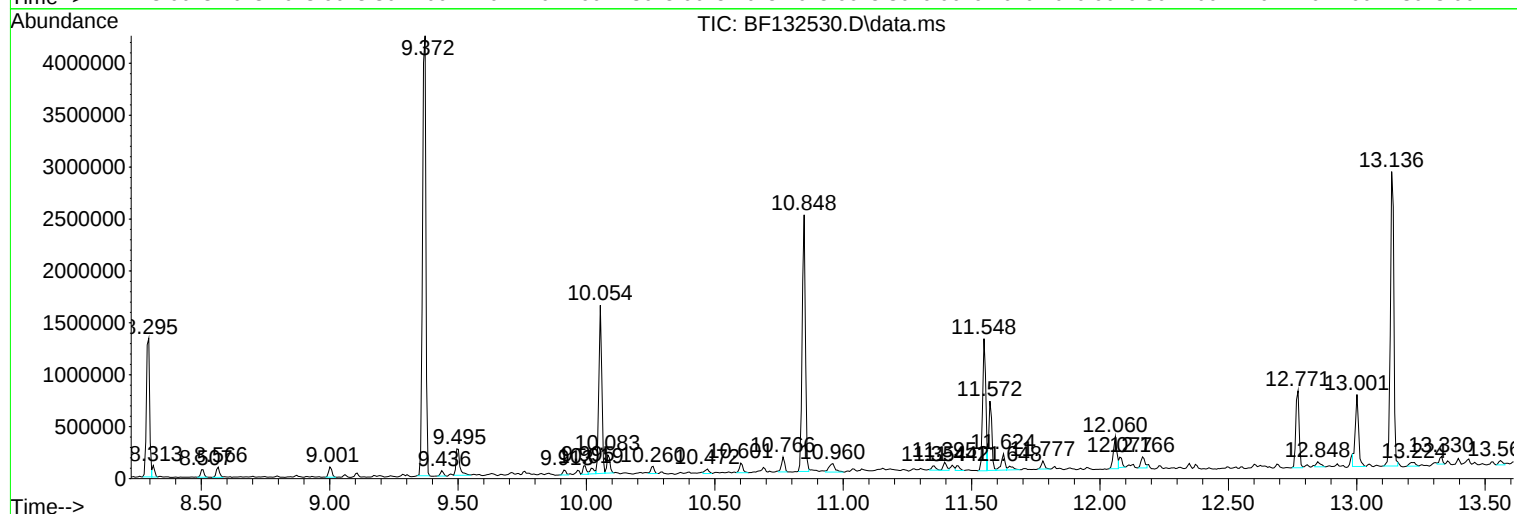
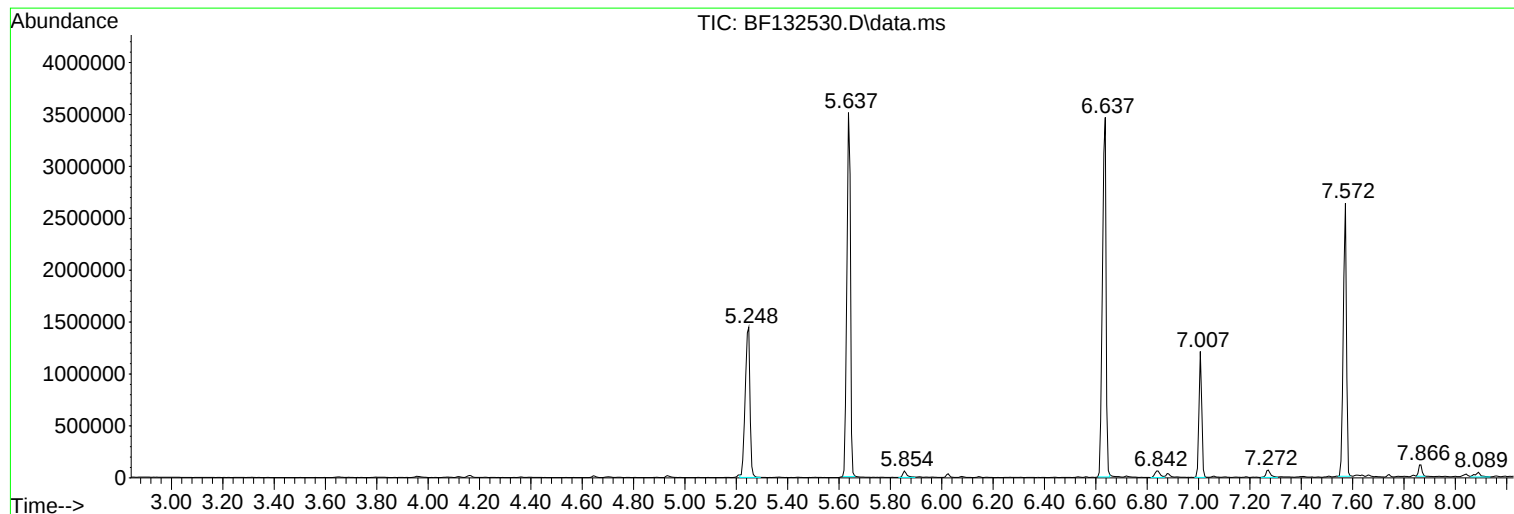
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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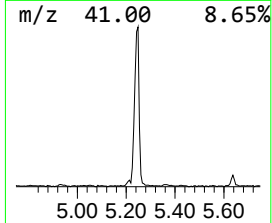
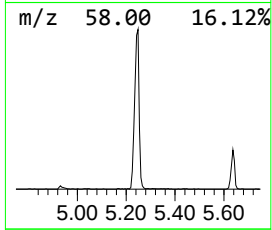
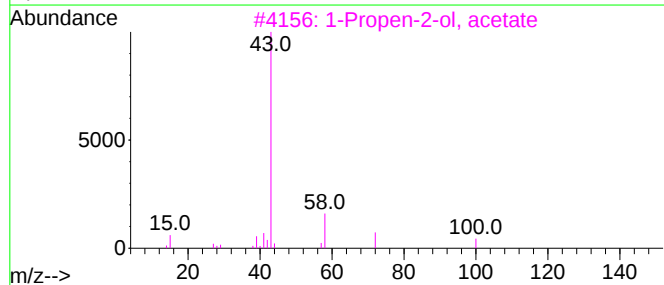
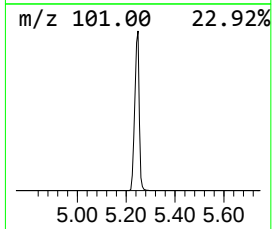
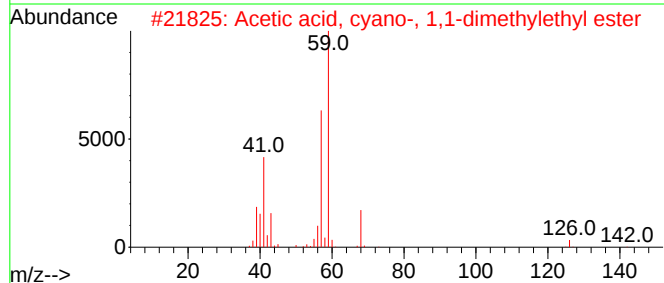
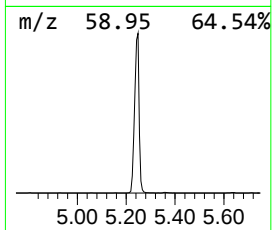
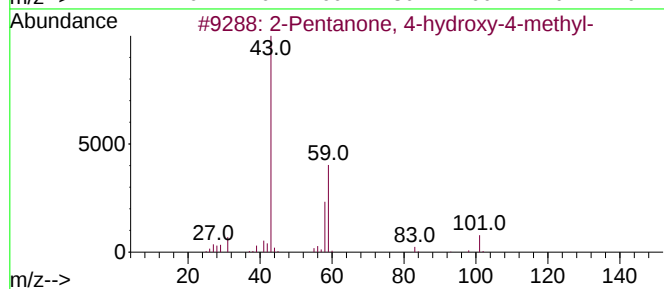
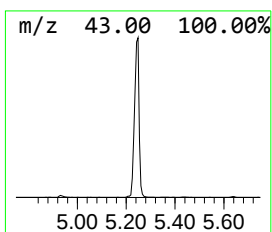
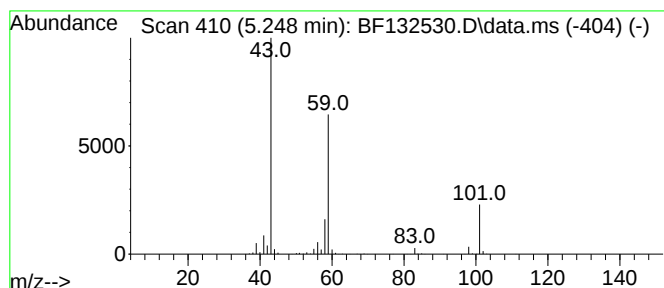
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.248	39.53 ng	1842720	1,4-Dichlorobenzene-d4	7.007

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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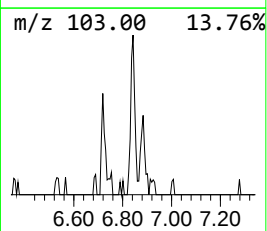
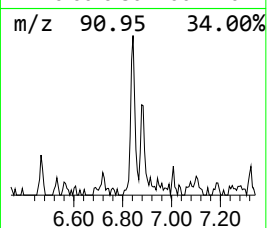
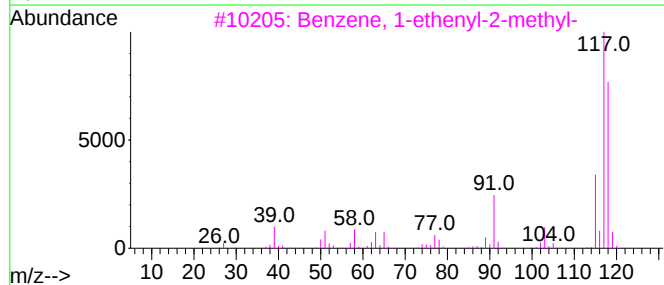
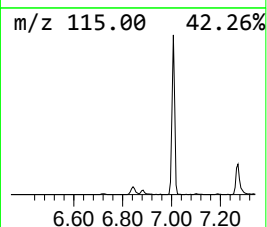
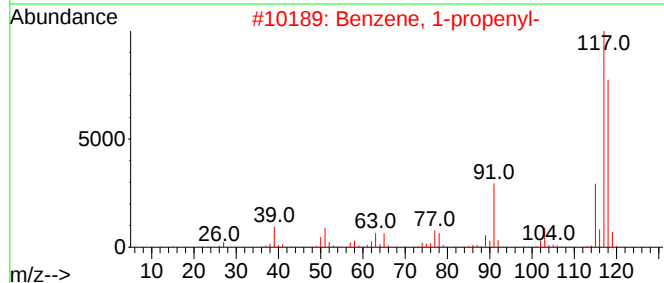
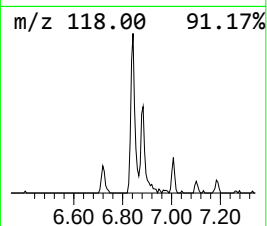
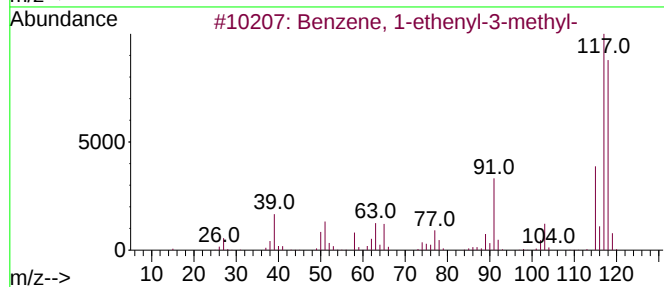
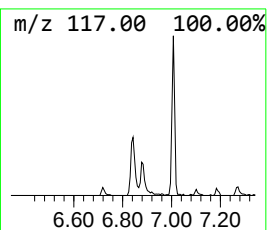
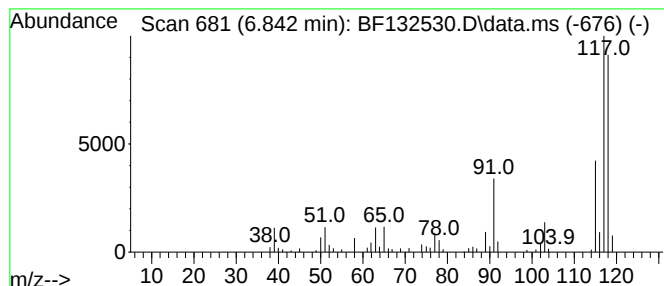
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-ethenyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.842	2.01 ng	93909	1,4-Dichlorobenzene-d4	7.007

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	97
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	95
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	94
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	93



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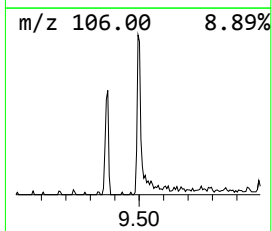
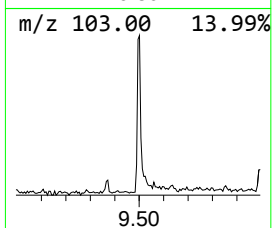
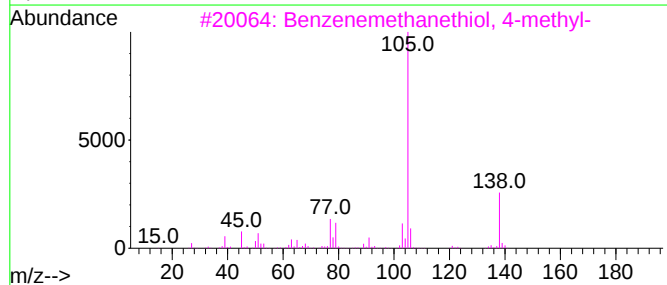
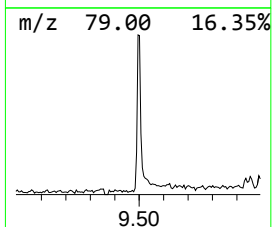
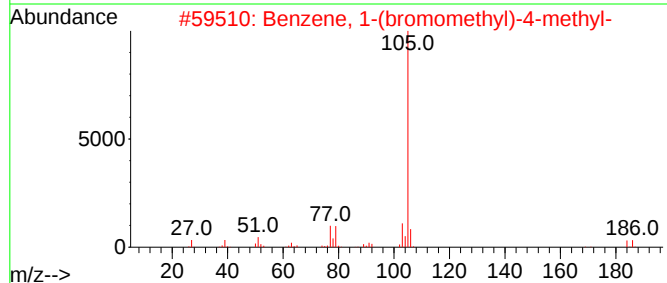
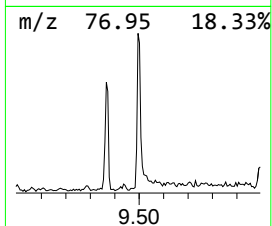
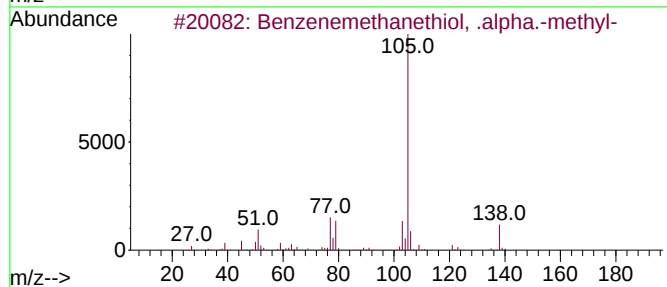
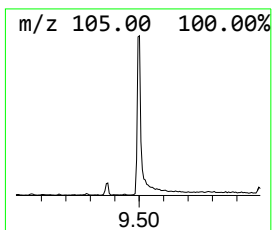
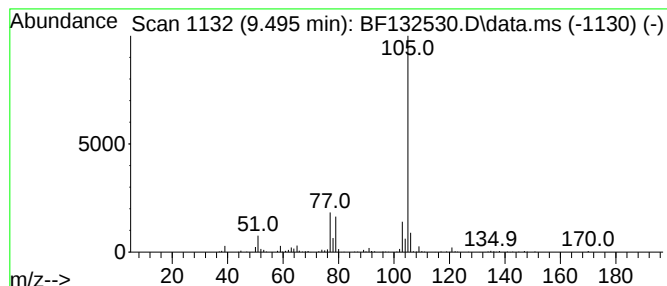
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzenemethanethiol, .alpha... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.495	4.14 ng	267702	Acenaphthene-d10	10.054

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenemethanethiol, .alpha.-met...	138	C8H10S	006263-65-6	91
2			Benzene, 1-(bromomethyl)-4-methyl-	184	C8H9Br	000104-81-4	78
3			Benzenemethanethiol, 4-methyl-	138	C8H10S	004498-99-1	78
4			2,4-Dimethylthiophenol	138	C8H10S	013616-82-5	72
5			2-Tolylloxirane	134	C9H10O	002783-26-8	72



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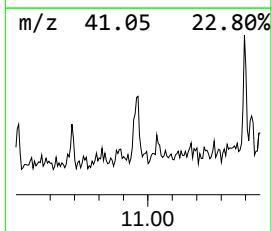
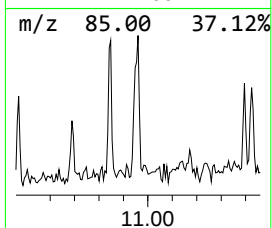
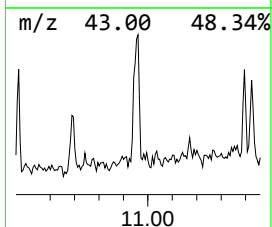
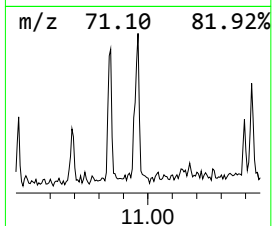
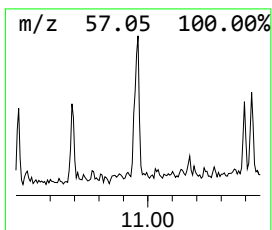
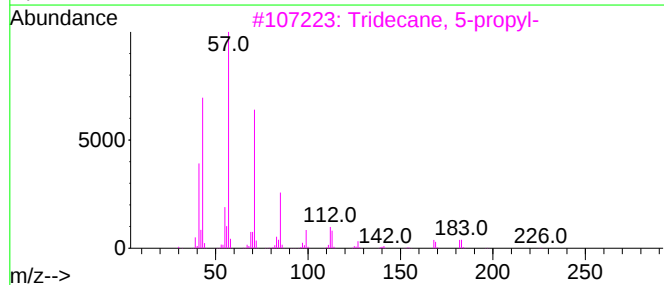
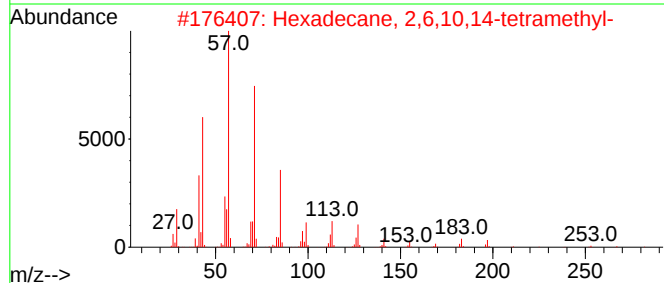
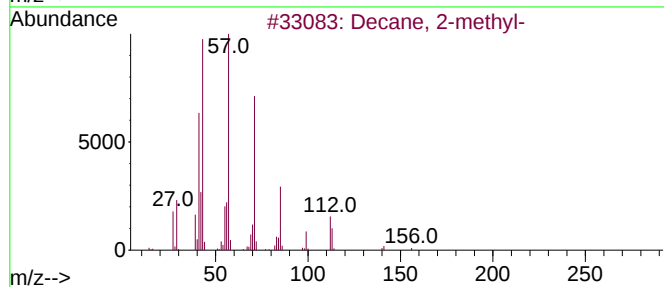
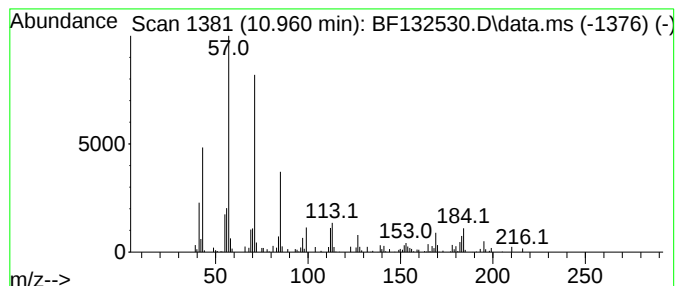
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Decane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.960	2.52 ng	137615	Phenanthrene-d10	11.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2-methyl-	156	C11H24	006975-98-0	87
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
3			Tridecane, 5-propyl-	226	C16H34	055045-11-9	80
4			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
5			Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	72



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ClientSampleId :
QAQC-COMP-2

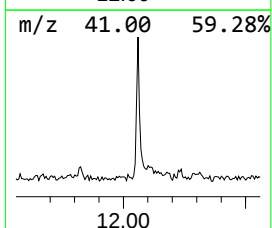
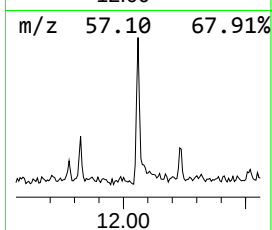
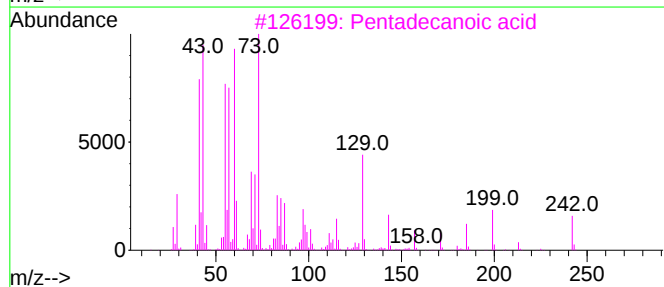
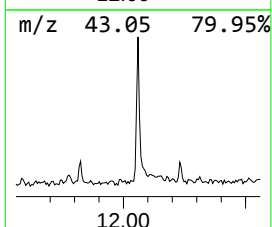
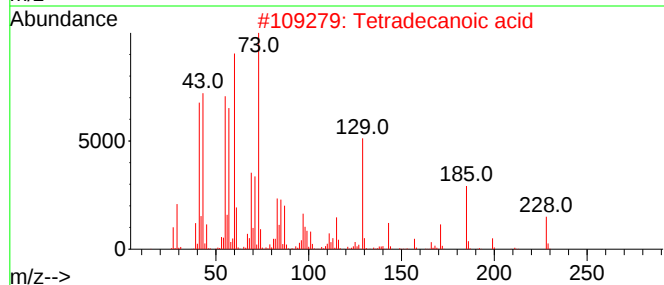
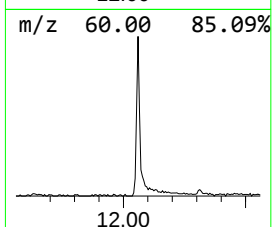
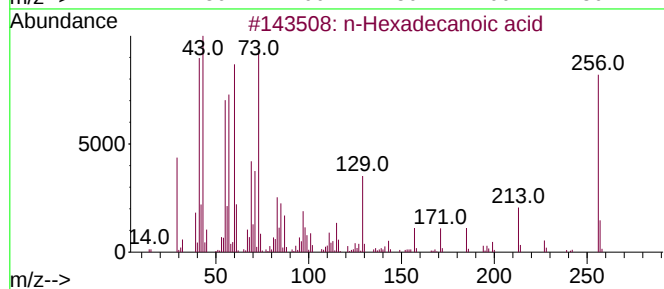
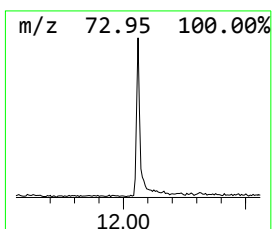
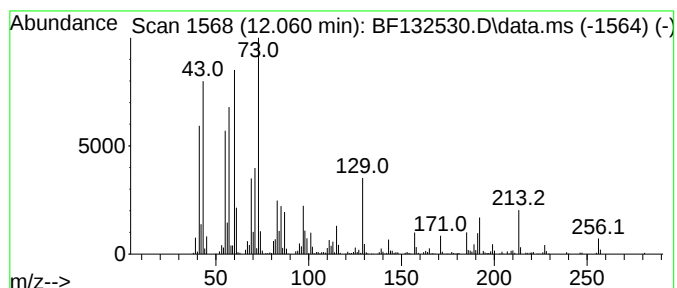
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	5.48 ng	299345	Phenanthrene-d10	11.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	97
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Dodecanoic acid	200	C12H24O2	000143-07-7	70
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022323\
Data File : BF132530.D
Acq On : 23 Feb 2023 20:24
Operator : CG\JU
Sample : 01659-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
QAQC-COMP-2

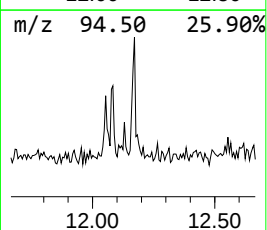
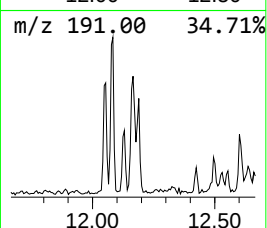
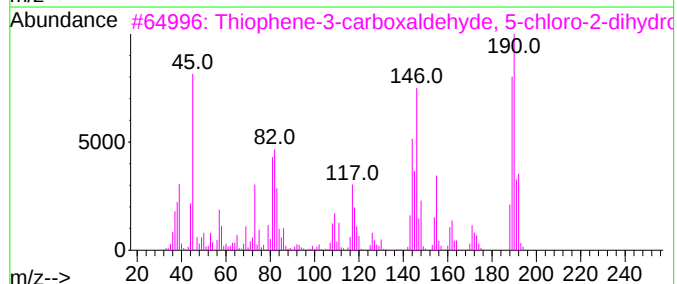
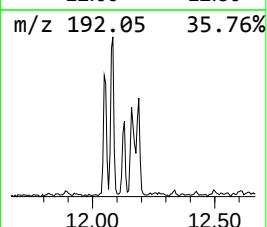
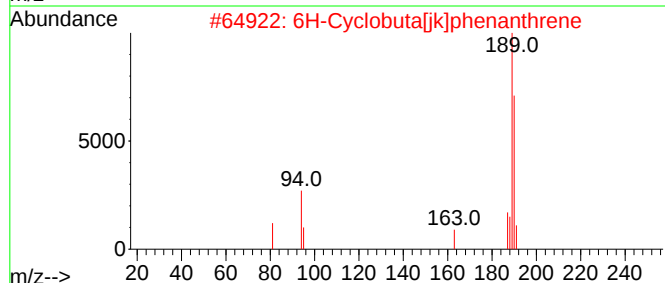
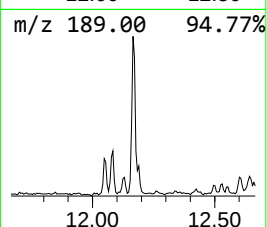
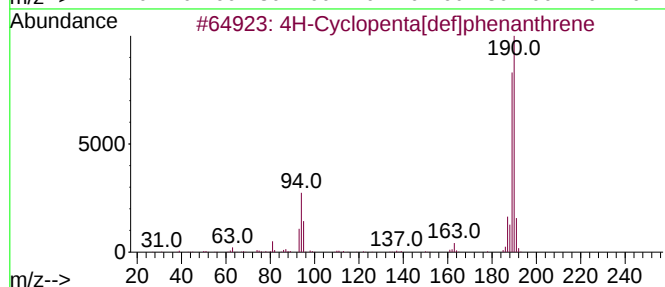
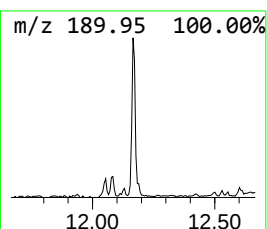
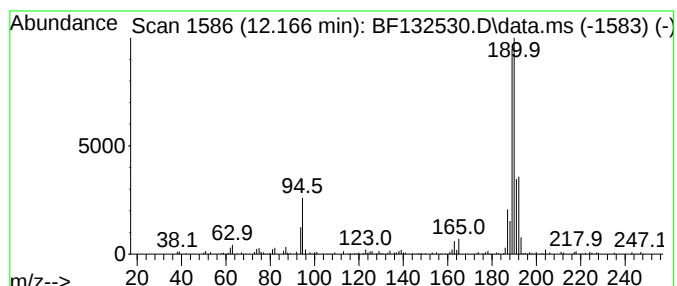
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.166	2.16 ng	117911	Phenanthrene-d10	11.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	74
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	49
4			1-(Phenylethynyl)-1H-1,2,3-benzo...	219	C14H9N3	209912-23-2	16
5			Methyl diselenide	190	C2H6Se2	007101-31-7	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022323\
Data File : BF132530.D
Acq On : 23 Feb 2023 20:24
Operator : CG\JU
Sample : 01659-01
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Instrument :
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ClientSampleId :
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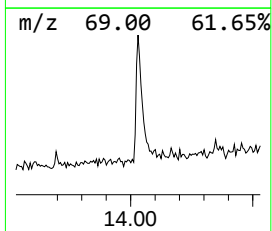
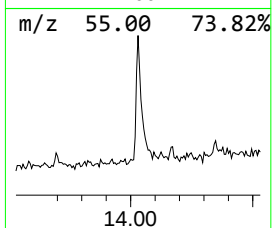
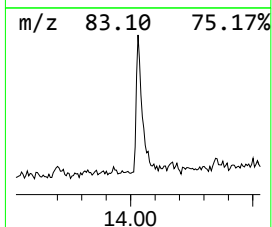
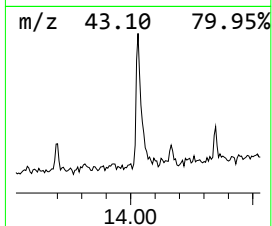
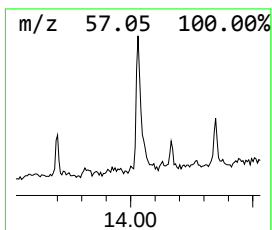
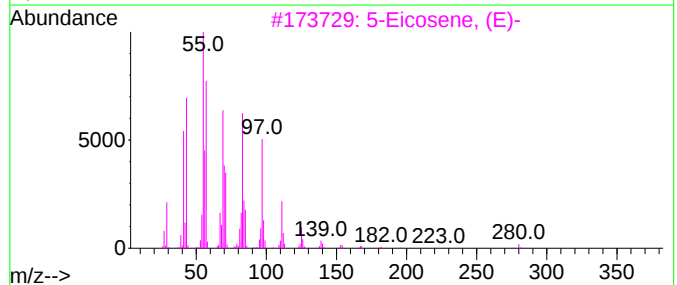
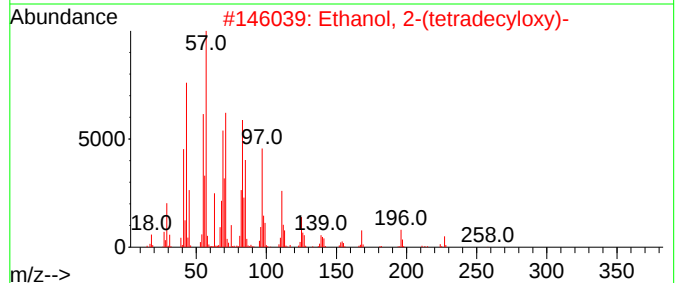
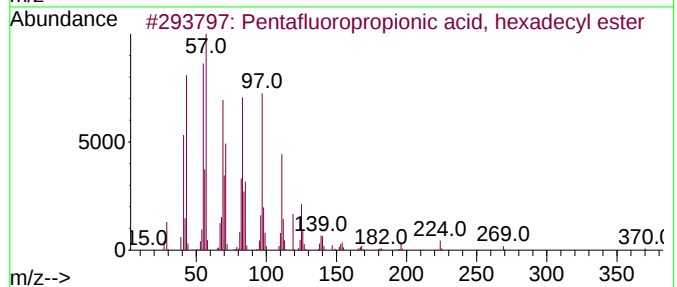
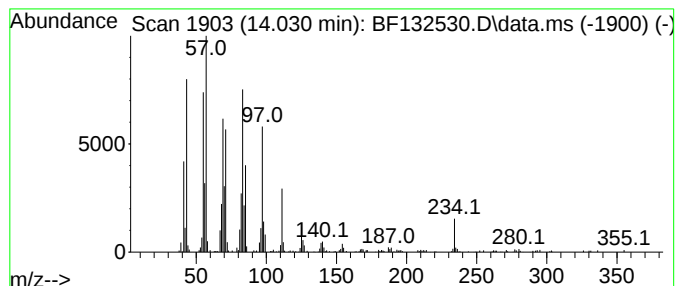
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.030	7.10 ng	412330	Chrysene-d12	14.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
3			5-Eicosene, (E)-	280	C20H40	074685-30-6	86
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	81
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022323\
Data File : BF132530.D
Acq On : 23 Feb 2023 20:24
Operator : CG\JU
Sample : 01659-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
QAQC-COMP-2

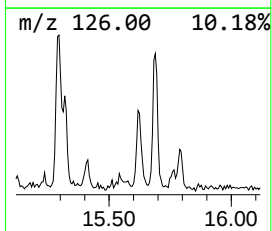
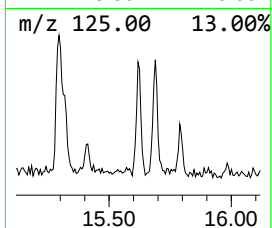
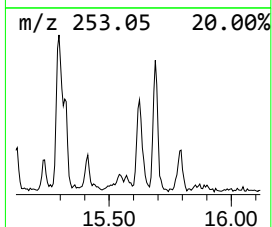
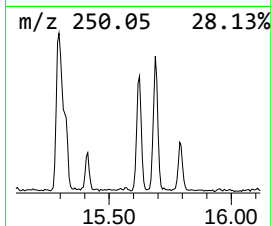
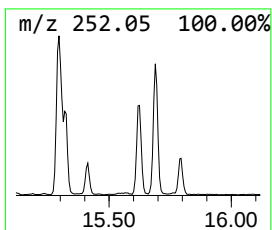
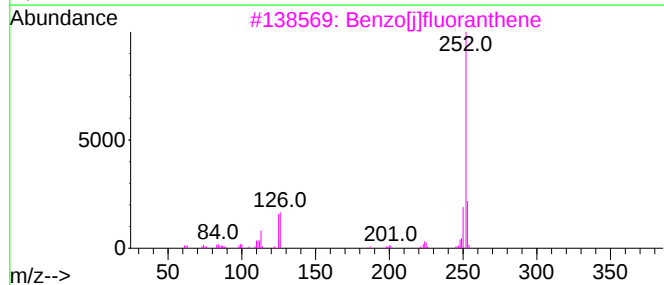
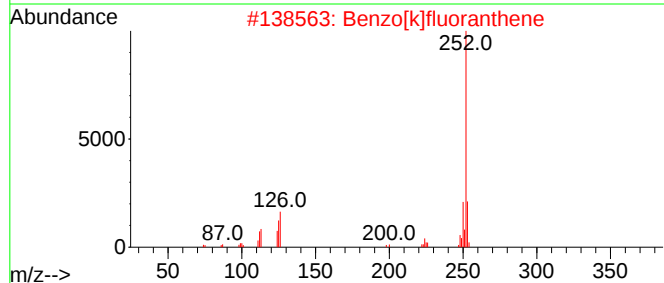
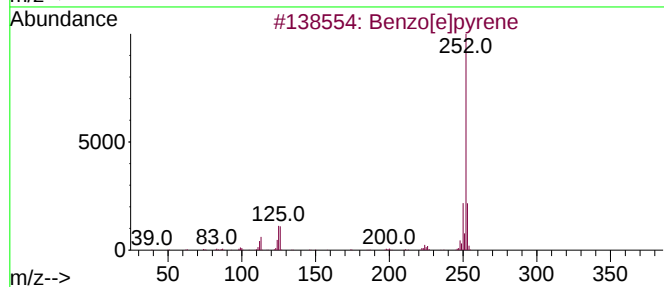
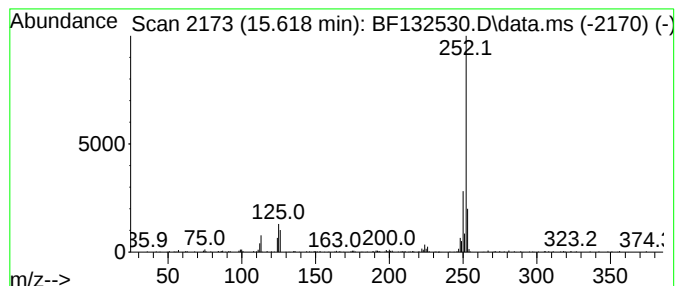
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.618	4.76 ng	205757	Perylene-d12	15.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	94
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	91
4			Benzo[a]pyrene	252	C20H12	000050-32-8	81
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022323\
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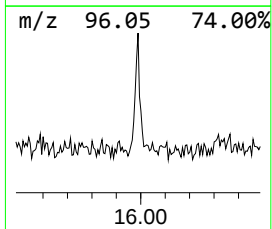
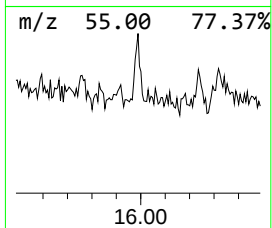
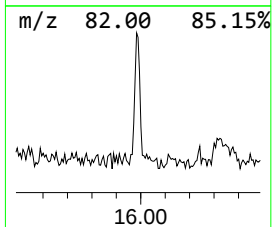
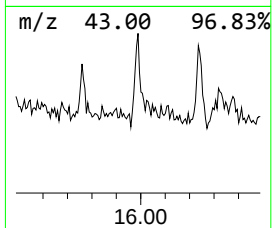
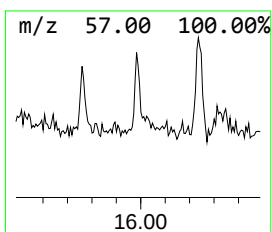
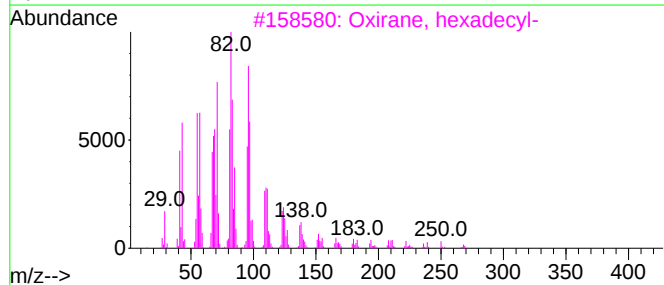
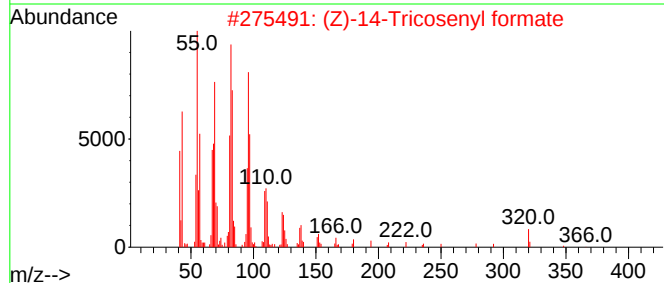
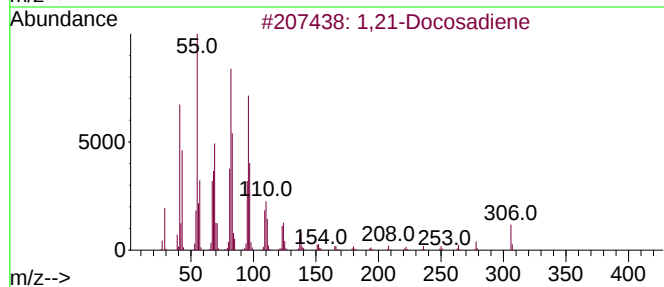
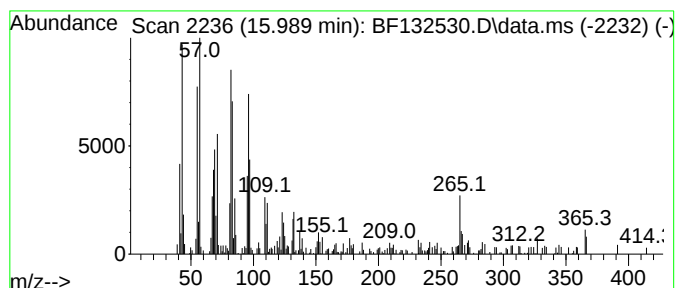
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 1,21-Docosadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.989	2.46 ng	106380	Perylene-d12	15.759	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,21-Docosadiene	306	C22H42	053057-53-7	92
2	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	64
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	62
4	1,19-Eicosadiene	278	C20H38	014811-95-1	53
5	Docosanal	324	C22H44O	057402-36-5	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022323\
Data File : BF132530.D
Acq On : 23 Feb 2023 20:24
Operator : CG\JU
Sample : 01659-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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-ethe...	6.842	2.0	ng	93909	1	7.007	932265	20.0
Benzenemethanet...	9.495	4.1	ng	267702	3	10.054	1294170	20.0
Decane, 2-methyl-	10.960	2.5	ng	137615	4	11.548	1092930	20.0
n-Hexadecanoic ...	12.060	5.5	ng	299345	4	11.548	1092930	20.0
4H-Cyclopenta[d]...	12.166	2.2	ng	117911	4	11.548	1092930	20.0
Pentafluoroprop...	14.030	7.1	ng	412330	5	14.207	1161320	20.0
Benzo[e]pyrene	15.618	4.8	ng	205757	6	15.759	865113	20.0
1,21-Docosadiene	15.989	2.5	ng	106380	6	15.759	865113	20.0