

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
 Data File : BF126184.D
 Acq On : 13 Nov 2021 23:41
 Operator : JU/CG
 Sample : M4573-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MBR1

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126184.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.445	360	401	403	rBV2	267064	2017163	12.76%	1.873%
2	4.669	412	439	441	rBV2	171904	862742	5.46%	0.801%
3	5.181	510	526	527	rBV4	132406	349708	2.21%	0.325%
4	5.451	568	572	575	rBV	1338285	1329291	8.41%	1.234%
5	5.634	589	603	608	rBV4	790691	2740703	17.33%	2.545%
6	5.892	622	647	650	rBV	615279	3141369	19.87%	2.917%
7	6.275	705	712	721	rVB2	192932	326866	2.07%	0.304%
8	6.457	739	743	747	rBV	1165839	1188602	7.52%	1.104%
9	6.516	747	753	761	rVB	289366	556774	3.52%	0.517%
10	6.828	803	806	810	rBV	1815777	1522543	9.63%	1.414%
11	6.910	816	820	825	rBV	116424	196964	1.25%	0.183%
12	6.998	826	835	836	rVV2	199324	400679	2.53%	0.372%
13	7.045	836	843	845	rVV5	366428	1030809	6.52%	0.957%
14	7.151	846	861	871	rVB	1280338	4463815	28.23%	4.145%
15	7.233	871	875	877	rBV	433094	452076	2.86%	0.420%
16	7.281	877	883	889	rVB	825957	1350619	8.54%	1.254%
17	7.392	895	902	905	rBV	4175137	3980814	25.18%	3.696%
18	7.575	930	933	941	rBV	1235140	1459430	9.23%	1.355%
19	7.645	941	945	951	rVB	218979	239764	1.52%	0.223%
20	7.869	973	983	1000	rBV2	353309	684587	4.33%	0.636%
21	8.028	1006	1010	1020	rBV	1577213	1697951	10.74%	1.577%
22	8.116	1020	1025	1028	rBV	2183770	1966474	12.44%	1.826%
23	8.333	1045	1062	1065	rBV5	272202	803799	5.08%	0.746%
24	8.404	1065	1074	1077	rVV	1158692	1947005	12.31%	1.808%
25	8.475	1083	1086	1096	rVB	164907	173083	1.09%	0.161%
26	8.822	1139	1145	1155	rBV	757506	894416	5.66%	0.830%
27	9.192	1203	1208	1211	rBV	8633728	7284019	46.07%	6.763%
28	9.310	1224	1228	1231	rVV	458768	405748	2.57%	0.377%
29	9.745	1298	1302	1304	rBV	1352128	1163023	7.36%	1.080%
30	9.769	1304	1306	1310	rVB	437011	369232	2.34%	0.343%
31	9.869	1319	1323	1326	rBV	2913520	2303794	14.57%	2.139%
32	10.369	1400	1408	1413	rBV	153675	197846	1.25%	0.184%
33	10.427	1413	1418	1428	rVB	360001	424454	2.68%	0.394%
34	10.545	1435	1438	1441	rVB	373150	272386	1.72%	0.253%
35	10.657	1449	1457	1460	rBV	2566314	2525967	15.98%	2.345%
36	10.839	1483	1488	1492	rBV	912614	918489	5.81%	0.853%

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37	11.051	1514	1524	1527	rBV	9468823	15811721	100.00%	14.681%
38	11.098	1527	1532	1537	rVV	3933125	3877641	24.52%	3.600%
39	11.157	1537	1542	1552	rVV	4934015	5360551	33.90%	4.977%
40	11.357	1571	1576	1579	rBV	2240286	1887186	11.94%	1.752%
41	11.786	1641	1649	1650	rBV	7303634	8822787	55.80%	8.192%
42	11.816	1652	1654	1656	rVV	8047317	5634666	35.64%	5.232%
43	11.845	1656	1659	1662	rVV	212399	209894	1.33%	0.195%
44	11.880	1662	1665	1672	rVV2	1361431	1320582	8.35%	1.226%
45	11.945	1673	1676	1684	rVB2	854135	972325	6.15%	0.903%
46	12.133	1704	1708	1709	rBV	717479	606160	3.83%	0.563%
47	12.151	1709	1711	1721	rVB2	1126027	948091	6.00%	0.880%
48	12.245	1724	1727	1731	rVB	901564	766648	4.85%	0.712%
49	12.457	1761	1763	1766	rVB	221327	158378	1.00%	0.147%
50	12.939	1841	1845	1848	rBV	5273837	4825122	30.52%	4.480%
51	13.174	1880	1885	1895	rBV2	385034	521583	3.30%	0.484%
52	13.862	1995	2002	2013	rBV2	212064	414267	2.62%	0.385%
53	13.992	2020	2024	2028	rVB	1521456	1319969	8.35%	1.226%
54	14.757	2150	2154	2156	rBV	238118	251529	1.59%	0.234%
55	15.456	2267	2273	2277	rBV	1247922	1545255	9.77%	1.435%
56	15.933	2349	2354	2358	rBV	109837	163763	1.04%	0.152%
57	16.433	2435	2439	2448	rVB	111730	196523	1.24%	0.182%
58	17.409	2600	2605	2616	rVB7	128110	282196	1.78%	0.262%
59	17.715	2653	2657	2666	rVB2	59813	158589	1.00%	0.147%

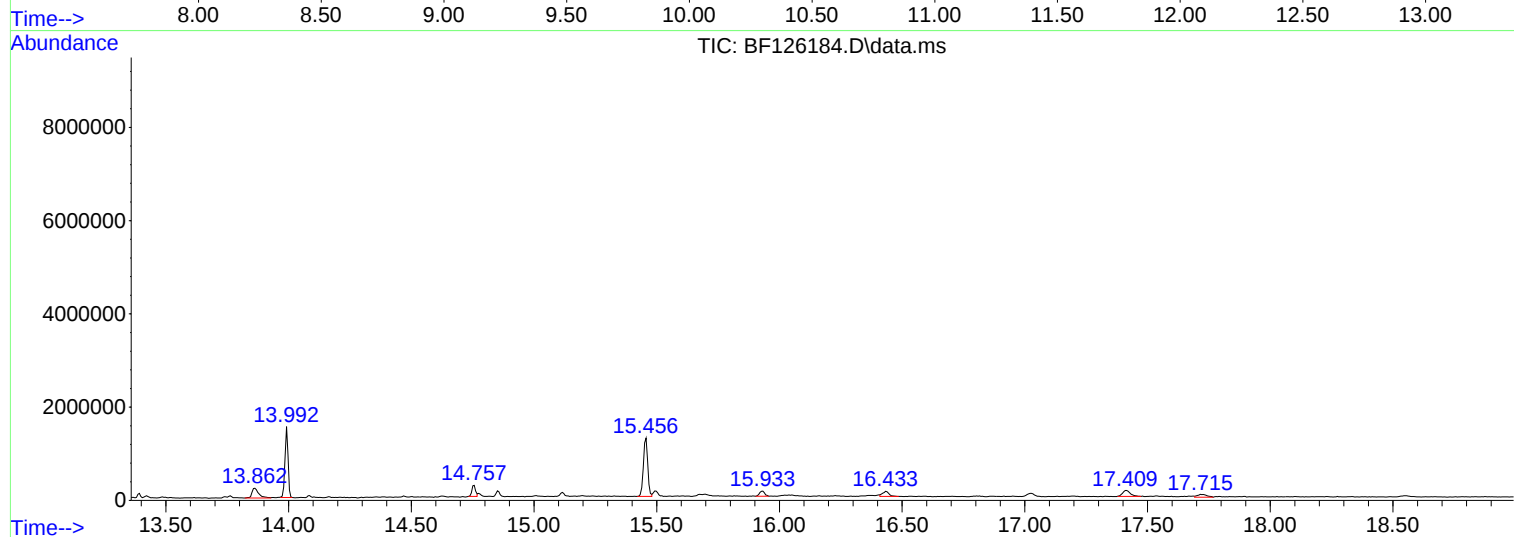
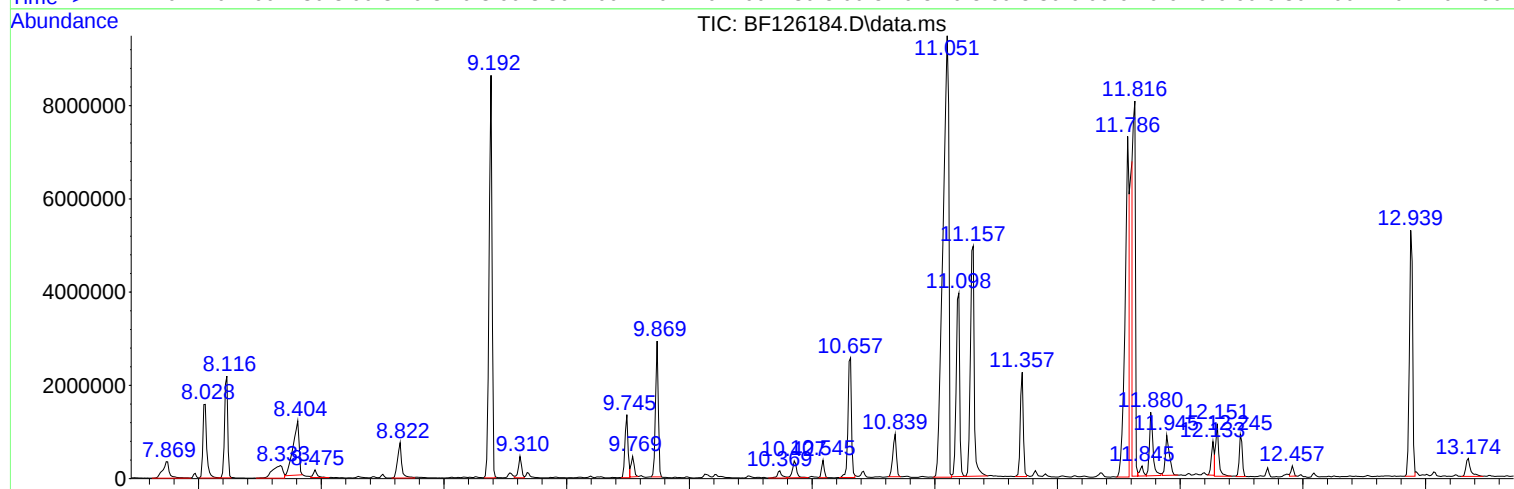
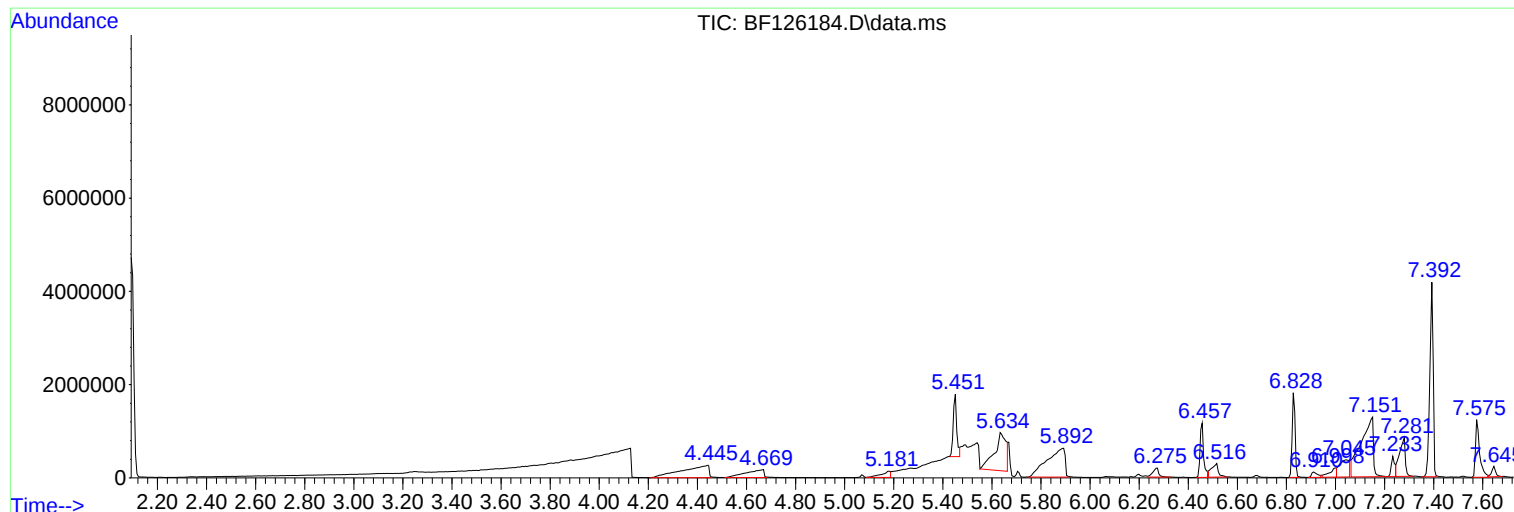
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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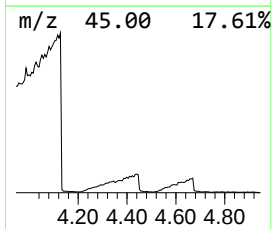
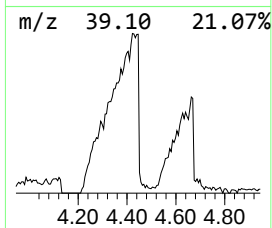
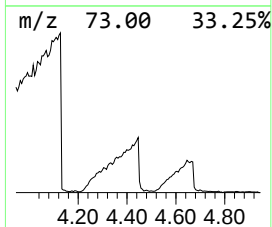
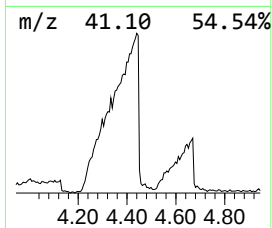
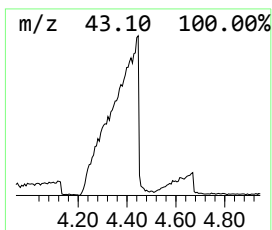
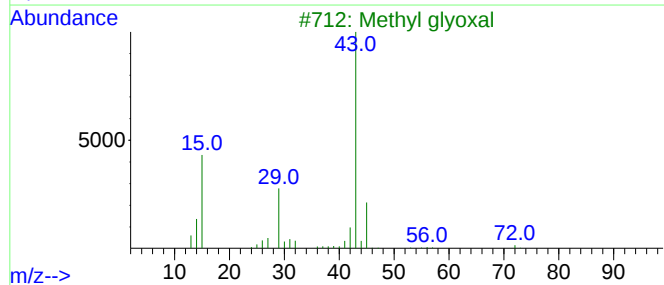
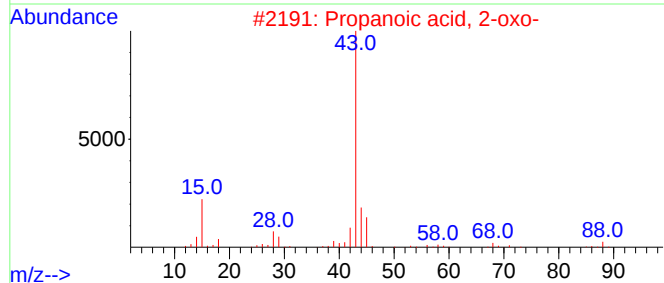
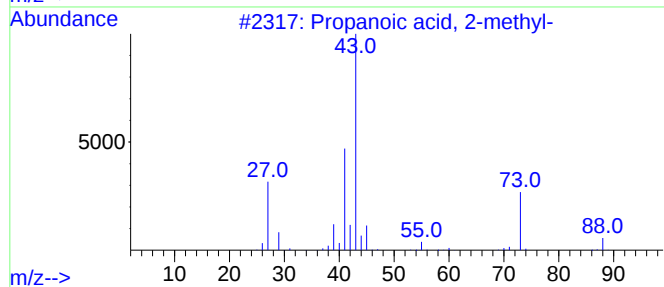
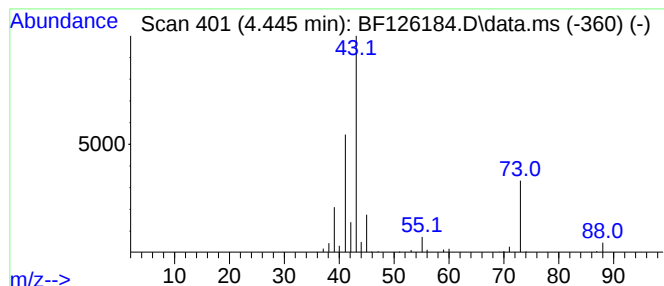
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.445	26.50 ng	2017160	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	86
2			Propanoic acid, 2-oxo-	88	C3H4O3	000127-17-3	38
3			Methyl glyoxal	72	C3H4O2	000078-98-8	23
4			Formic acid, 2-methylpropyl ester	102	C5H10O2	000542-55-2	17
5			Isobutyl nitrite	103	C4H9NO2	000542-56-3	10



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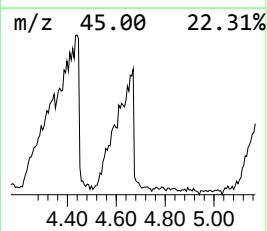
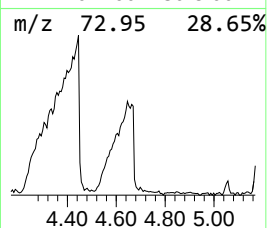
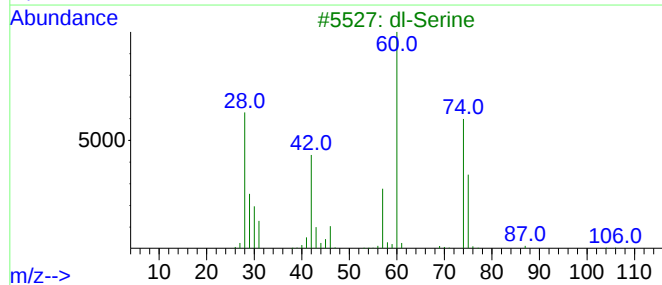
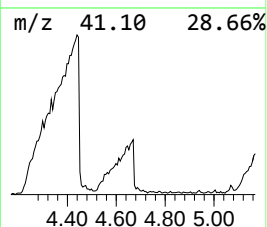
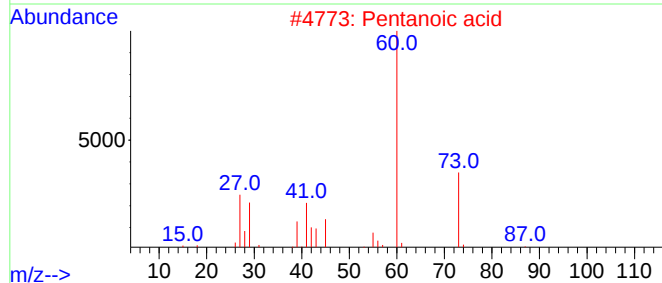
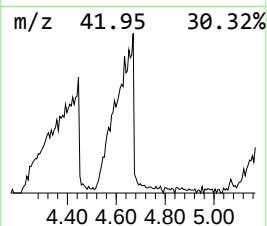
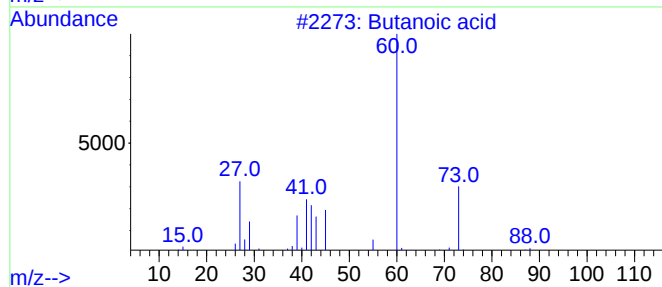
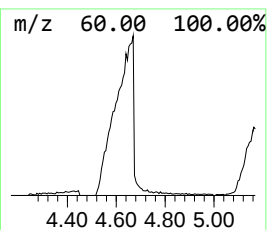
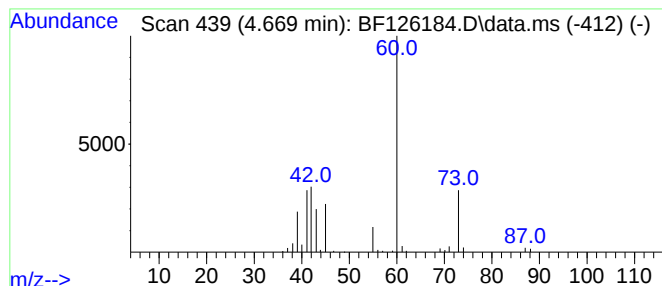
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Butanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.669	11.33 ng	862742	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	83
2			Pentanoic acid	102	C5H10O2	000109-52-4	38
3			dl-Serine	105	C3H7NO3	000302-84-1	36
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5			4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9



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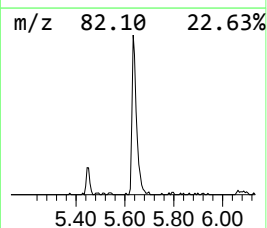
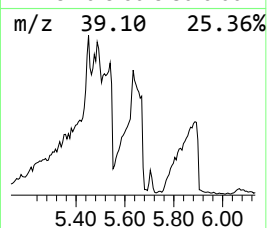
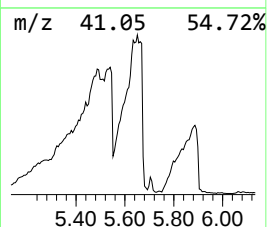
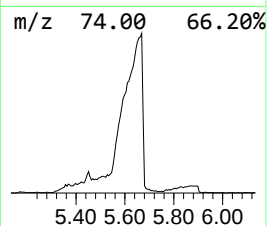
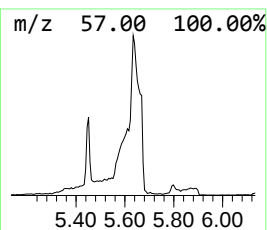
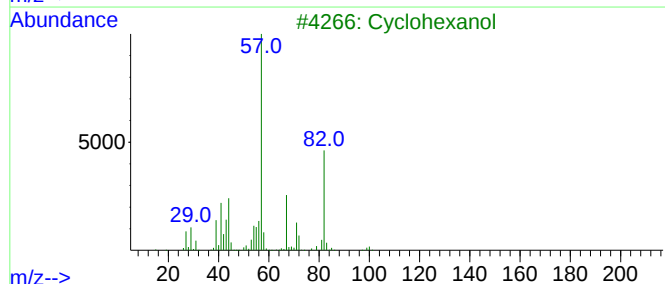
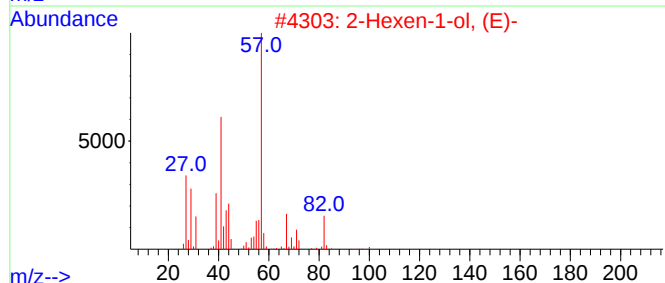
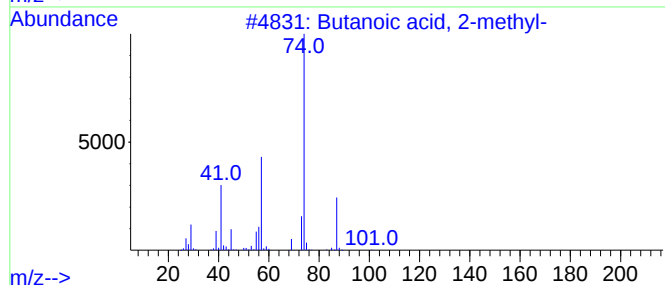
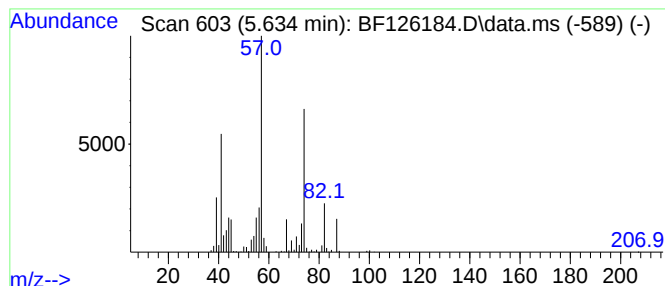
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown5.634 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.634	36.00 ng	2740700	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	38
2			2-Hexen-1-ol, (E)-	100	C6H12O	000928-95-0	38
3			Cyclohexanol	100	C6H12O	000108-93-0	30
4			Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	25
5			Cyclopentanol, 2-methyl-	100	C6H12O	024070-77-7	25



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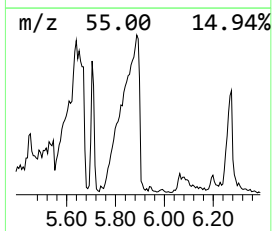
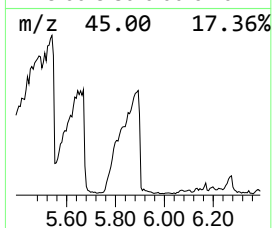
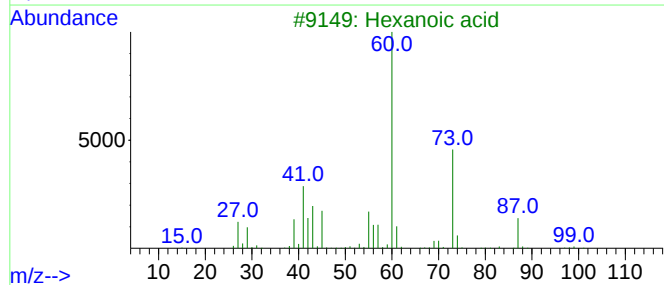
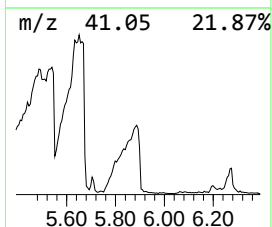
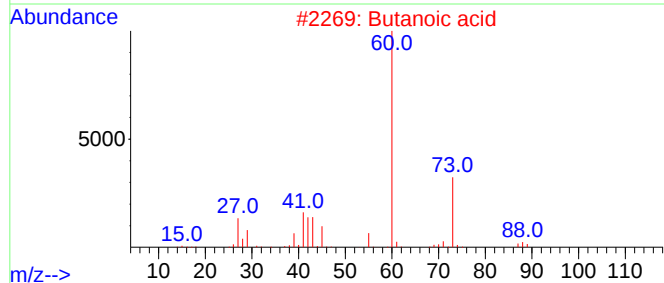
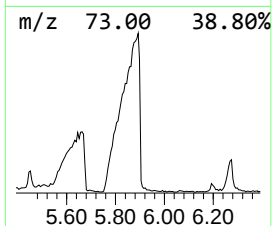
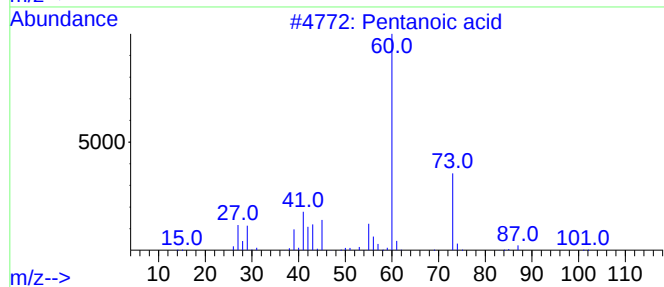
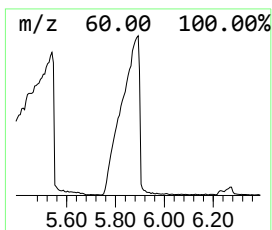
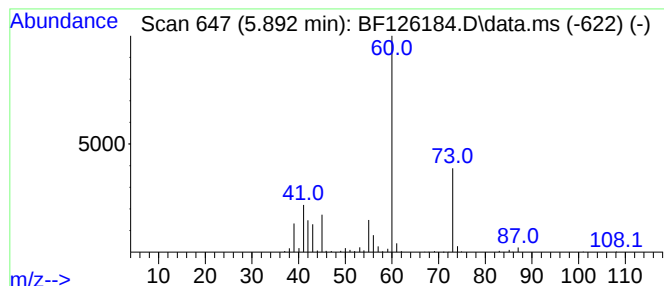
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.892	41.26 ng	3141370	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid	102	C5H10O2	000109-52-4	83
2			Butanoic acid	88	C4H8O2	000107-92-6	78
3			Hexanoic acid	116	C6H12O2	000142-62-1	64
4			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	59
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	45



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MBR1

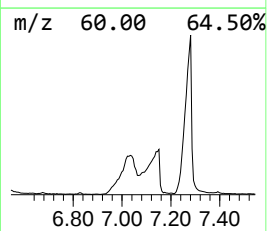
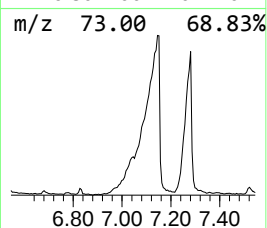
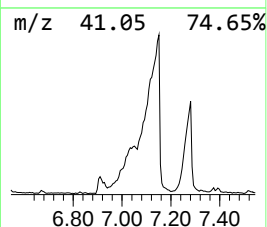
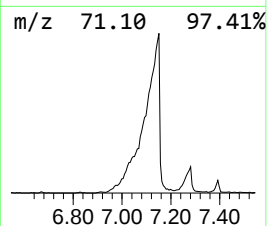
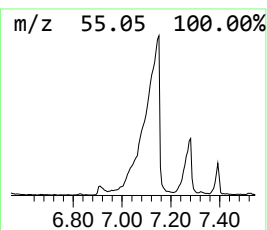
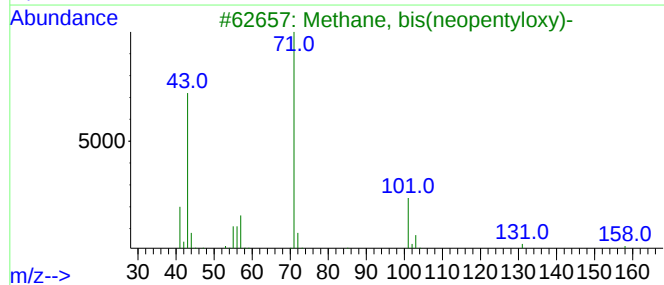
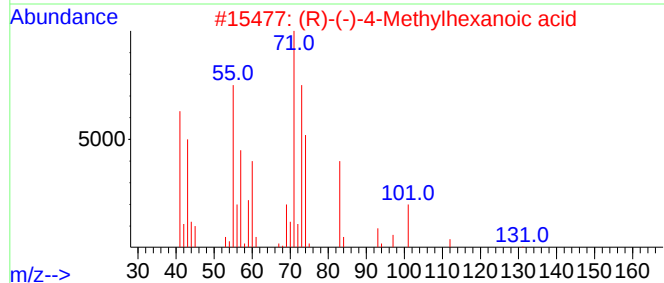
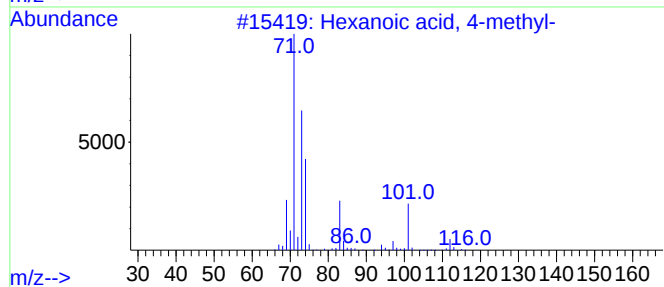
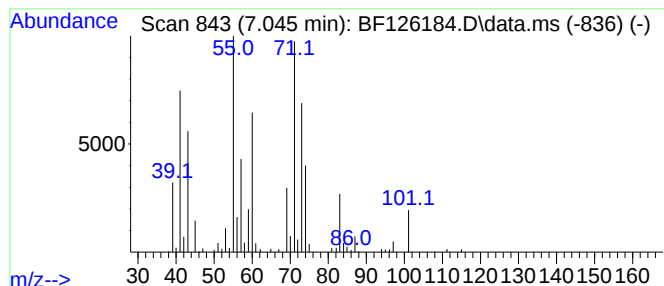
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexanoic acid, 4-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.045	13.54 ng	1030810	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 4-methyl-	130	C7H14O2	001561-11-1	83
2			(R)-(-)-4-Methylhexanoic acid	130	C7H14O2	052745-93-4	38
3			Methane, bis(neopentyloxy)-	188	C11H24O2	004457-17-4	12
4			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	12
5			2-Propenamide	71	C3H5NO	000079-06-1	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
Operator : JU/CG
Sample : M4573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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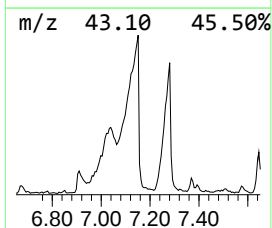
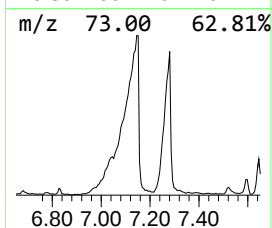
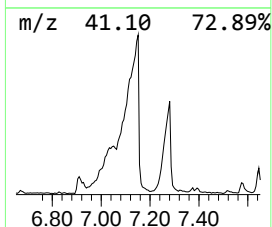
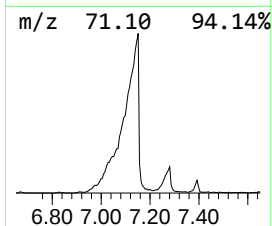
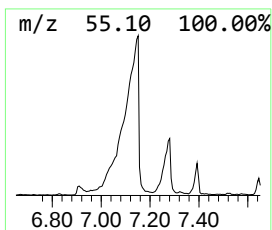
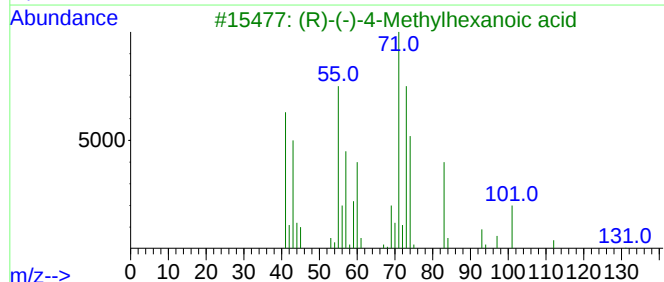
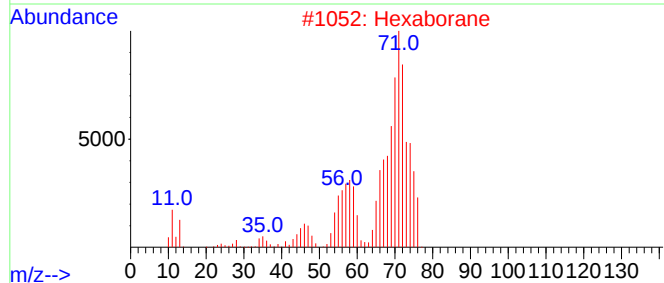
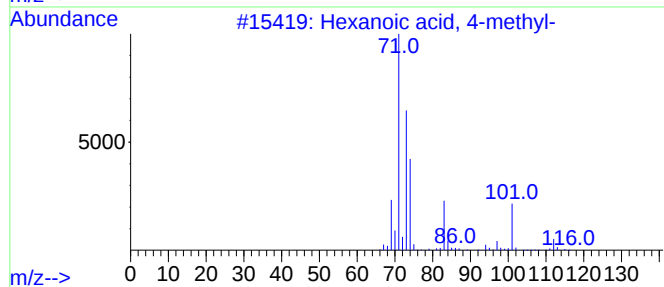
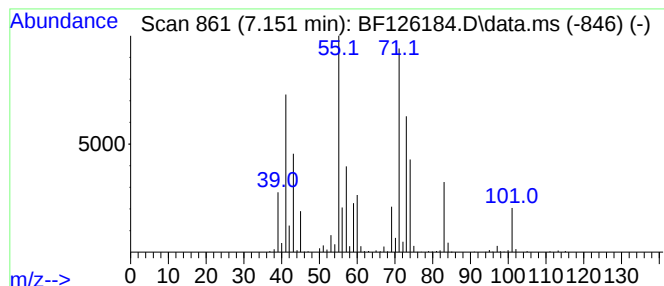
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown7.151 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.151	58.64 ng	4463820	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 4-methyl-	130	C7H14O2	001561-11-1	74
2			Hexaborane	76	B6H10	023777-80-2	38
3			(R)-(-)-4-Methylhexanoic acid	130	C7H14O2	052745-93-4	25
4			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	14
5			Oxirane, 3-hydroxypropyl-	102	C5H10O2	021915-56-0	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
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Sample : M4573-01
Misc :
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Instrument :
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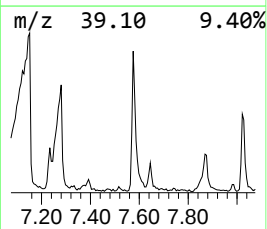
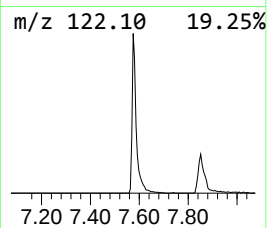
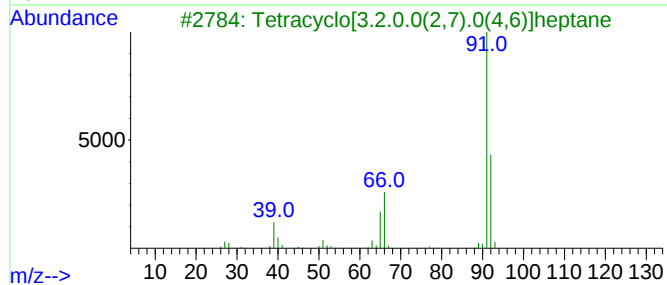
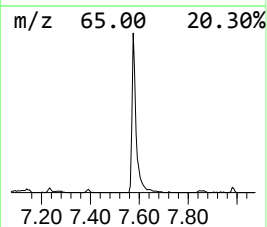
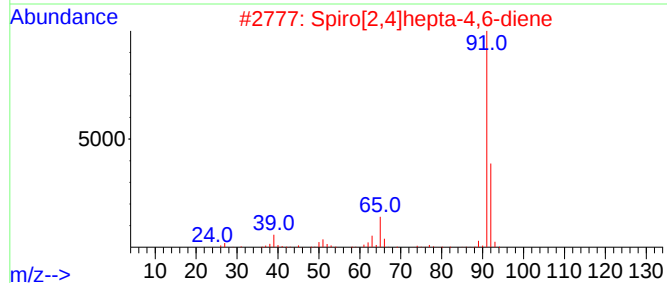
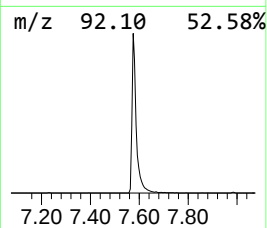
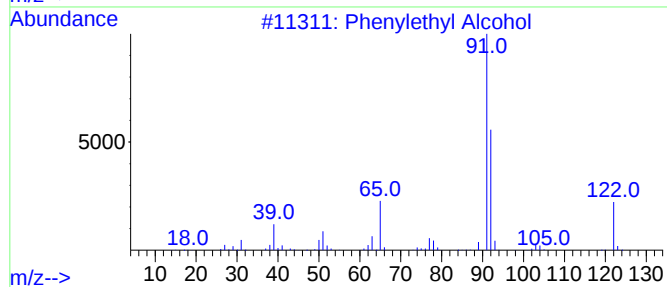
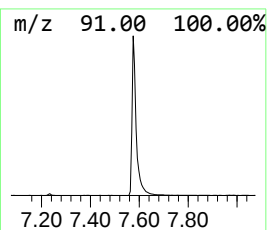
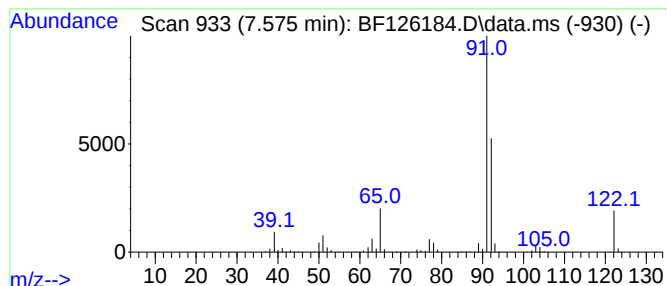
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenylethyl Alcohol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.575	14.84 ng	1459430	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenylethyl Alcohol	122	C8H10O	000060-12-8	97
2			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	76
3			Tetracyclo[3.2.0.0(2,7).0(4,6)]h...	92	C7H8	000278-06-8	64
4			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	64
5			2,5-Norbornadiene	92	C7H8	000121-46-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
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Sample : M4573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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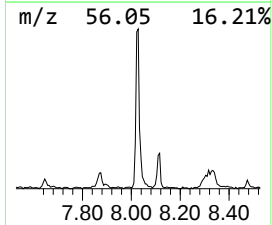
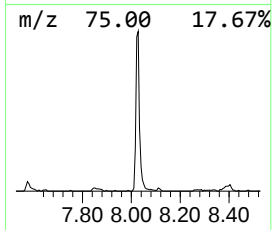
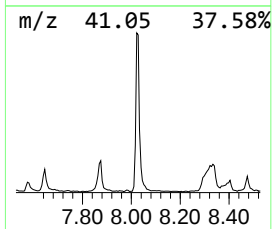
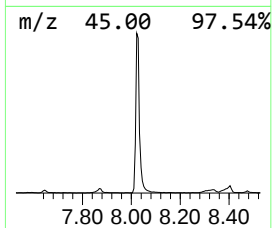
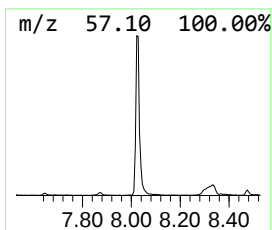
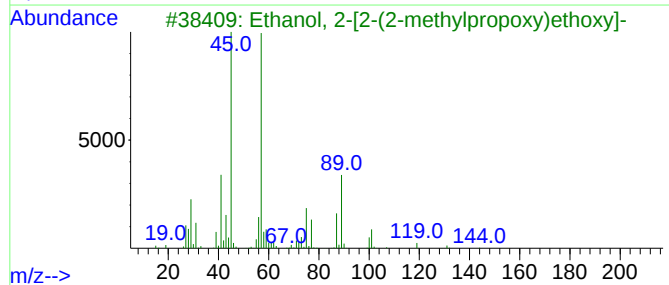
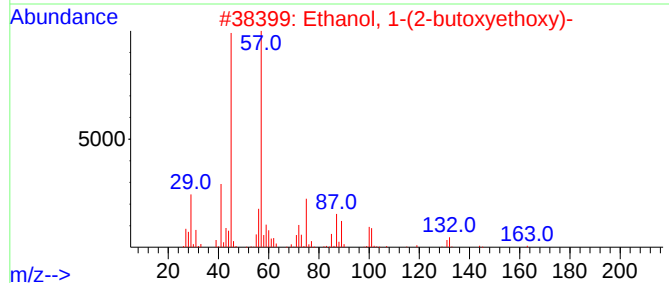
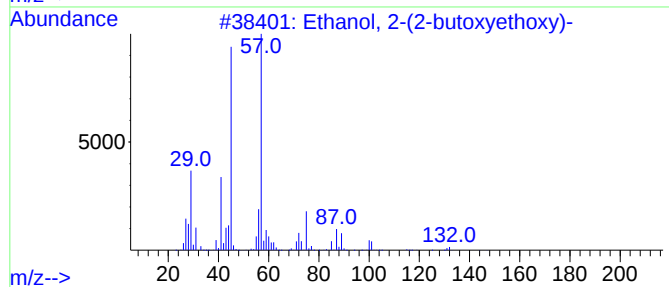
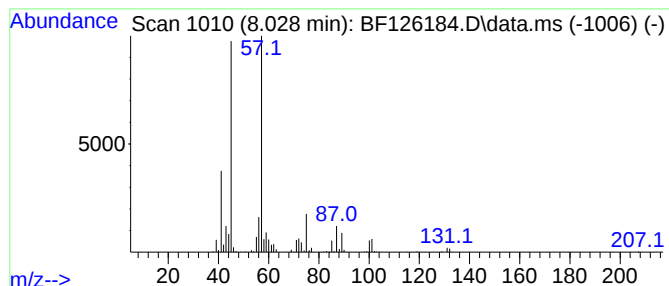
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.028	17.27 ng	1697950	Naphthalene-d8	8.116

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	78
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
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Sample : M4573-01
Misc :
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Instrument :
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ClientSampleId :
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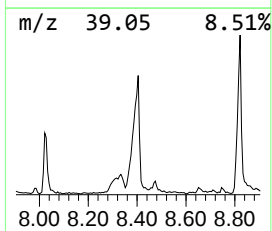
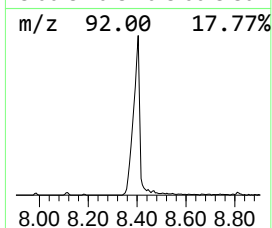
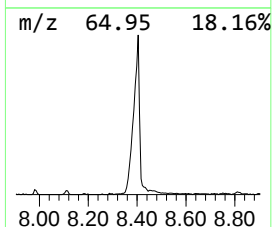
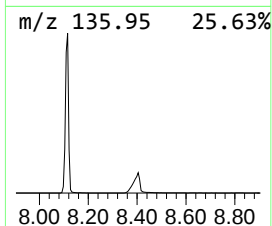
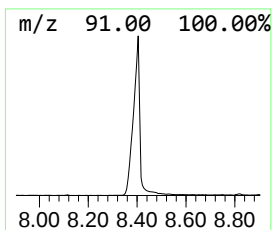
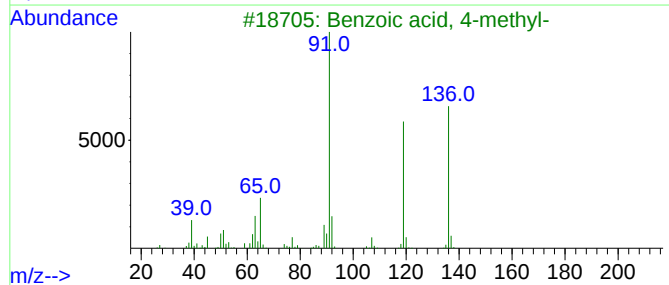
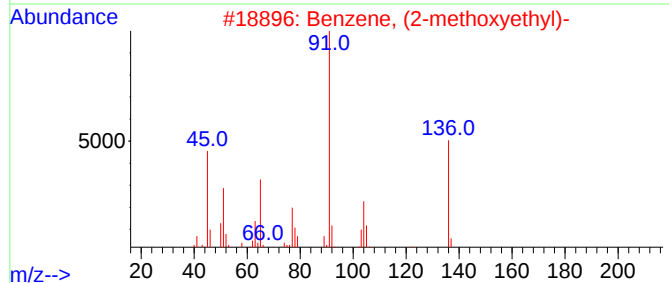
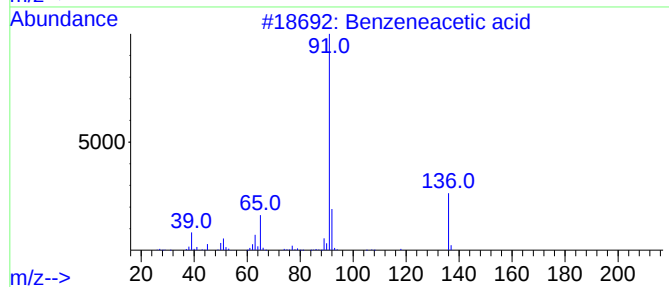
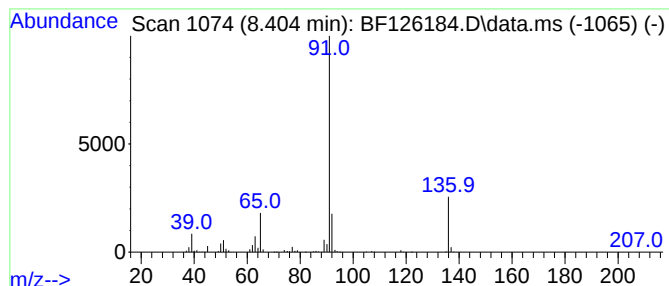
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzeneacetic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.404	19.80 ng	1947010	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	95
2			Benzene, (2-methoxyethyl)-	136	C9H12O	003558-60-9	72
3			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	59
4			Benzeneacetaldehyde	120	C8H8O	000122-78-1	50
5			Benzyl 2-chloroethyl sulfone	218	C9H11ClO2S	066998-67-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
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Sample : M4573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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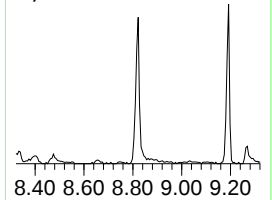
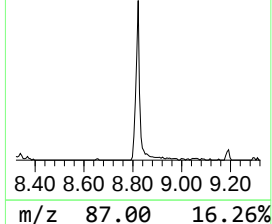
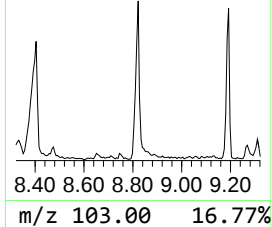
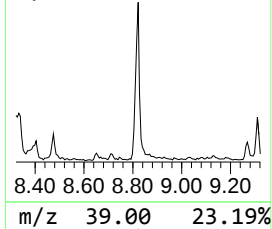
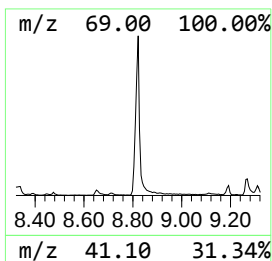
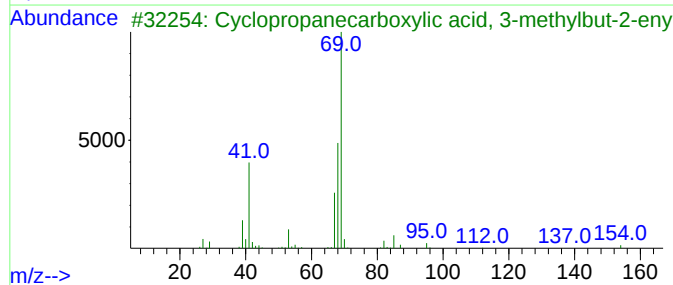
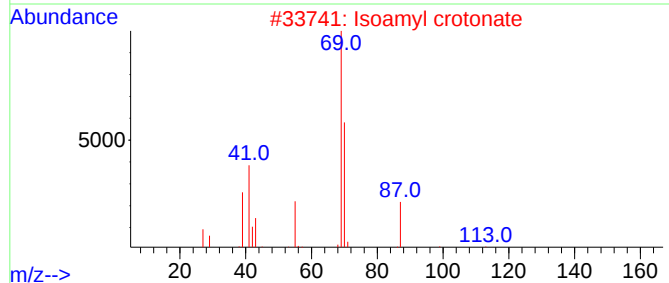
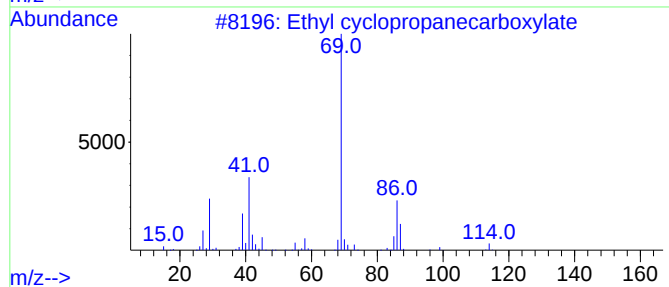
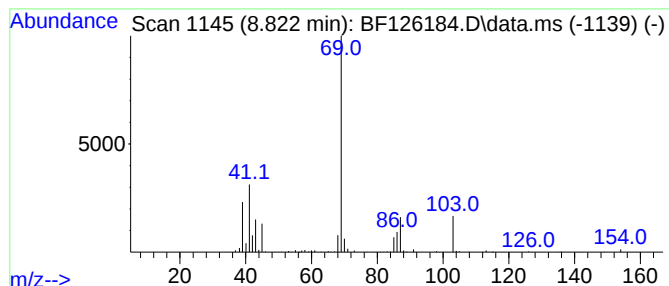
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown8.822 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.822	9.10 ng	894416	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
2			Isoamyl crotonate	156	C9H16O2	1010429-17-3	33
3			Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	33
4			(+)-3-hydroxybutyric acid, trif...	200	C6H7F3O4	1010374-31-1	9
5			1,6-Hexanediamine	116	C6H16N2	000124-09-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
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ALS Vial : 20 Sample Multiplier: 1

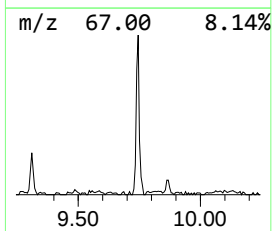
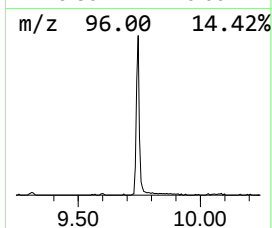
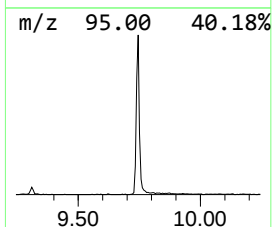
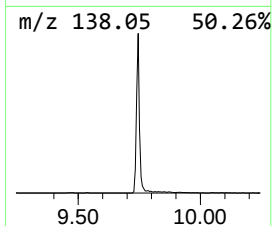
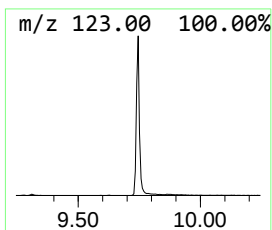
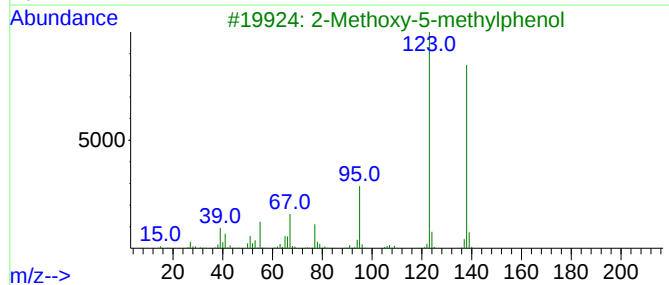
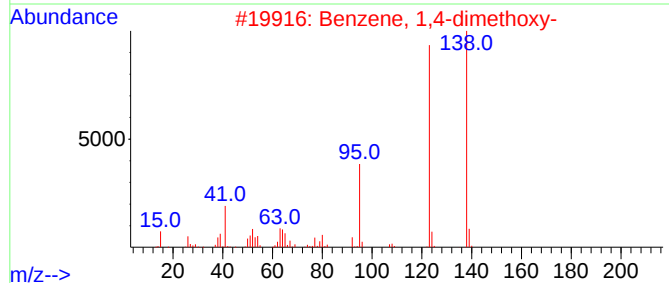
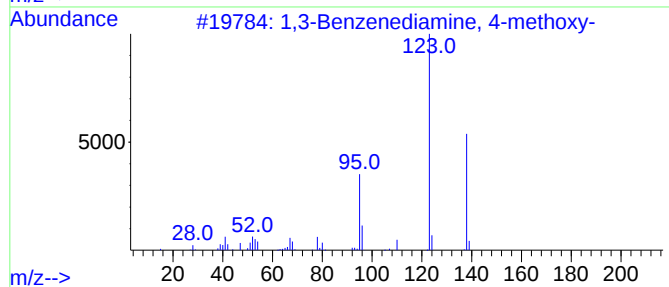
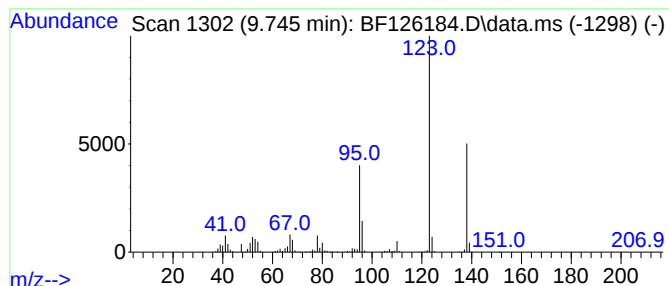
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1,3-Benzenediamine, 4-methoxy- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.745	10.10 ng	1163020	Acenaphthene-d10			9.869
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	96
2		Benzene, 1,4-dimethoxy-	138	C8H10O2	000150-78-7	78
3		2-Methoxy-5-methylphenol	138	C8H10O2	001195-09-1	72
4		Ethyl p-hydroxybenzoate	138	C8H10O2	002349-70-4	58
5		Benzene, 2-fluoro-1,3,5-trimethyl-	138	C9H11F	000392-69-8	52



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Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
Operator : JU/CG
Sample : M4573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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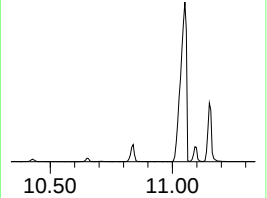
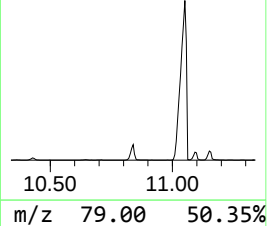
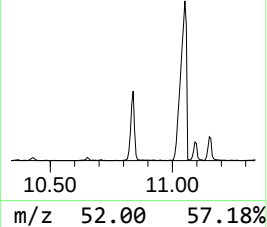
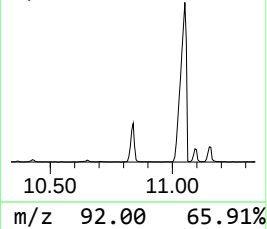
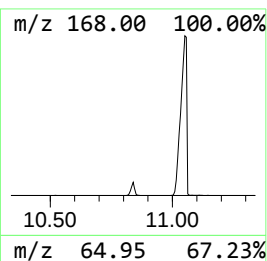
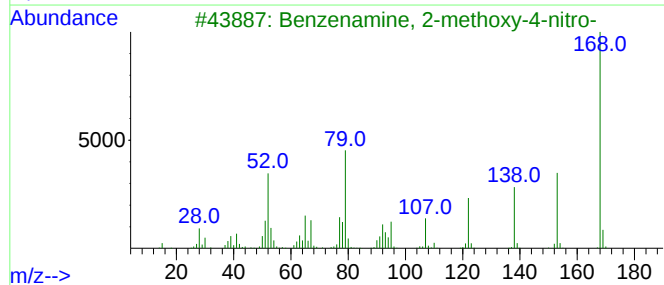
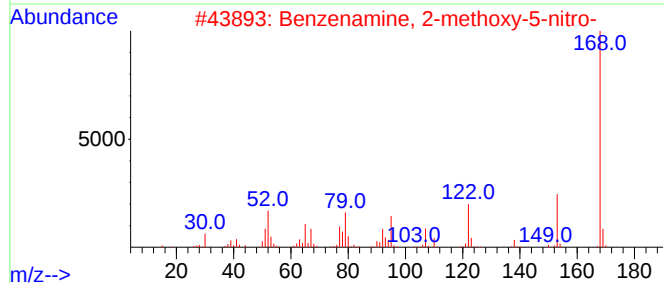
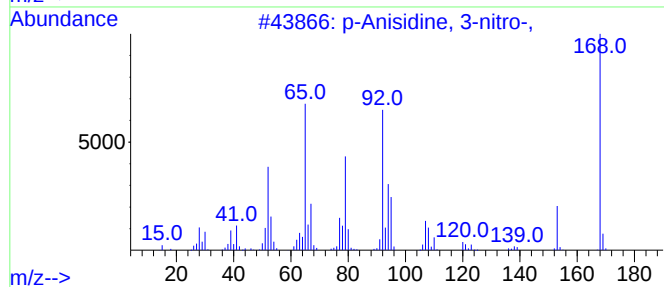
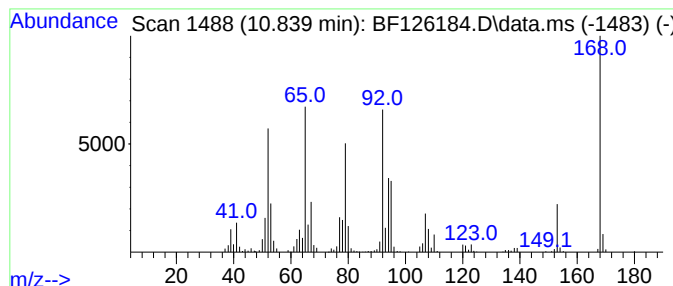
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 p-Anisidine, 3-nitro-, Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.839	9.73 ng	918489	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Anisidine, 3-nitro-,	168	C7H8N2O3	000577-72-0	98
2			Benzenamine, 2-methoxy-5-nitro-	168	C7H8N2O3	000099-59-2	32
3			Benzenamine, 2-methoxy-4-nitro-	168	C7H8N2O3	000097-52-9	27
4			Pyridine, 4-methyl-2-nitro-	138	C6H6N2O2	018368-71-3	25
5			Phenol, 4-methoxy-3-(methoxymeth...	168	C9H12O3	059907-65-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
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Sample : M4573-01
Misc :
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ClientSampleId :
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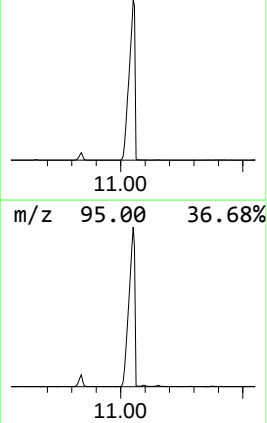
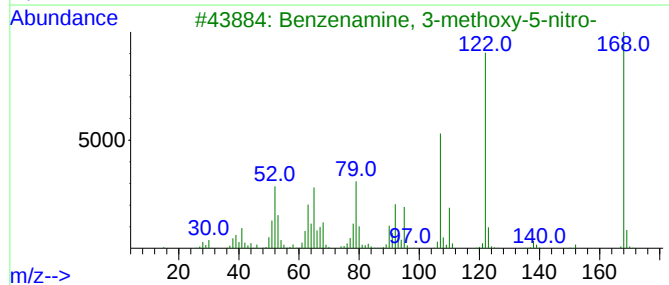
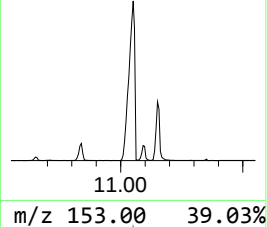
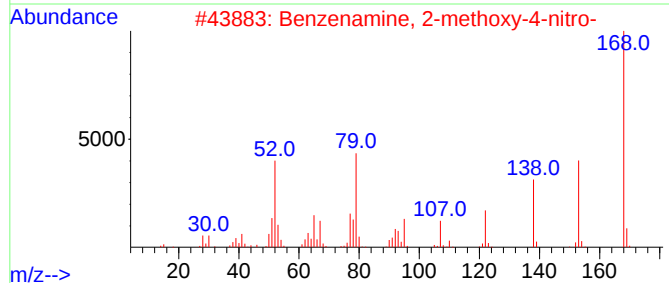
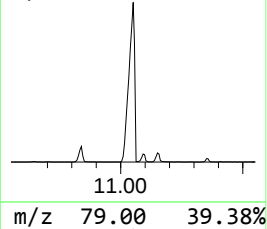
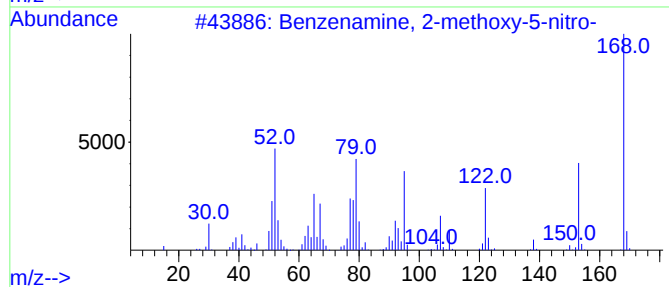
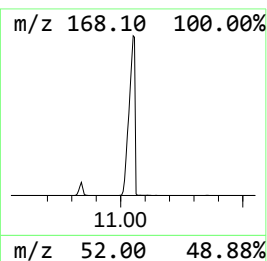
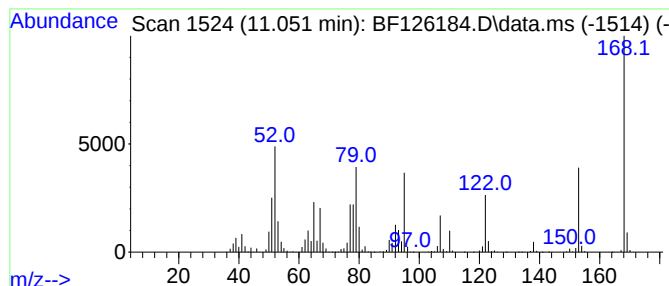
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzenamine, 2-methoxy-5-ni... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.051	167.57 ng	15811700	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenamine, 2-methoxy-5-nitro-	168	C7H8N2O3	000099-59-2	98
2			Benzenamine, 2-methoxy-4-nitro-	168	C7H8N2O3	000097-52-9	86
3			Benzenamine, 3-methoxy-5-nitro-	168	C7H8N2O3	000586-10-7	68
4			p-Anisidine, 3-nitro-,	168	C7H8N2O3	000577-72-0	64
5			Benzenamine, 4-methoxy-2-nitro-	168	C7H8N2O3	000096-96-8	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
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Sample : M4573-01
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ClientSampleId :
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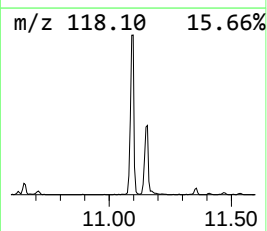
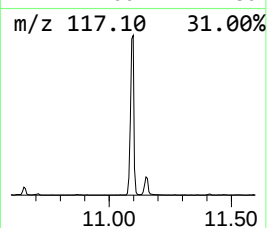
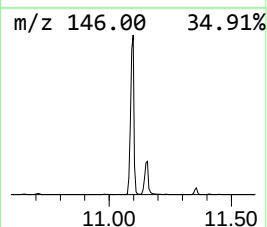
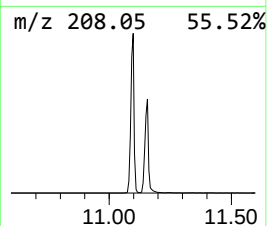
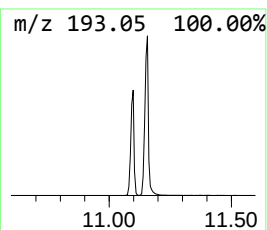
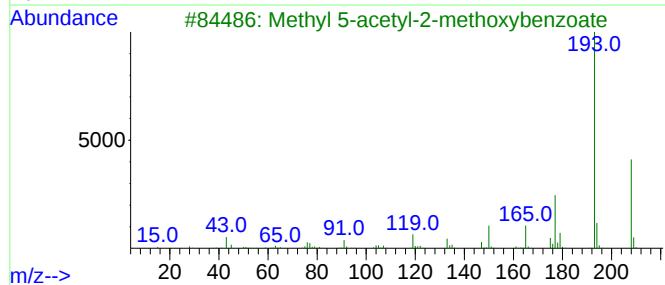
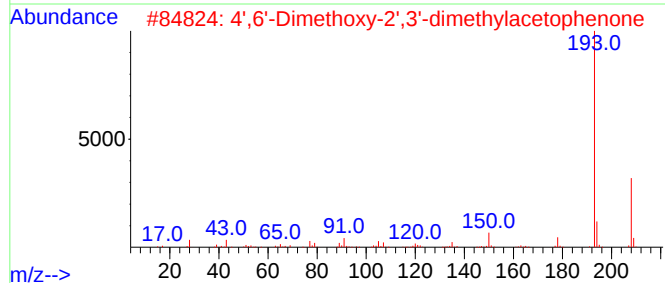
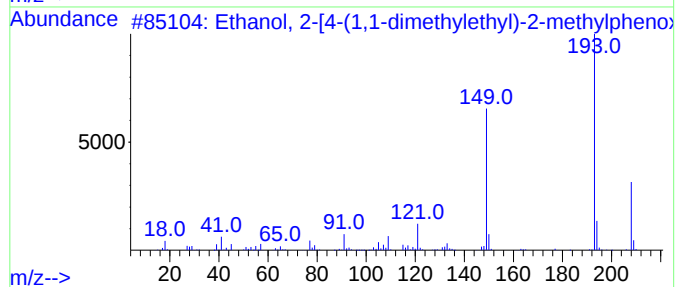
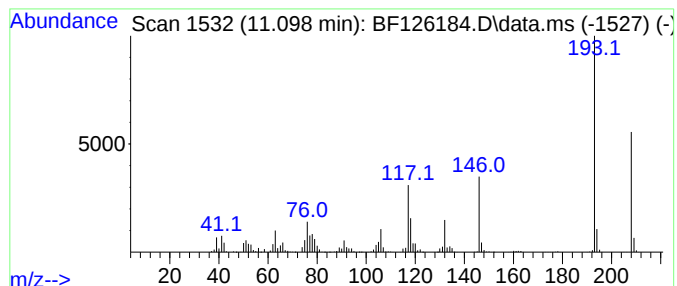
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown11.098 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.098	41.09 ng	3877640	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-[4-(1,1-dimethylethyl)-2-methylpheno	208	C13H20O2	054934-87-1	49
2			4',6'-Dimethoxy-2',3'-dimethylacetophenone	208	C12H16O3	1010244-80-3	49
3			Methyl 5-acetyl-2-methoxybenzoate	208	C11H12O4	039971-36-3	49
4			Benzaldehyde, 2-hydroxy-4-diethyl-	208	C11H16N2O2	198280-97-6	47
5			2-Acetylthiophene, 5-(2-thienyl)-	208	C10H8OS2	003515-18-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
Operator : JU/CG
Sample : M4573-01
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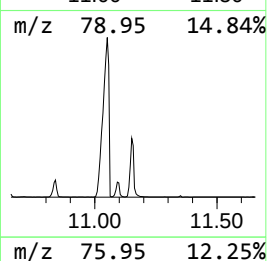
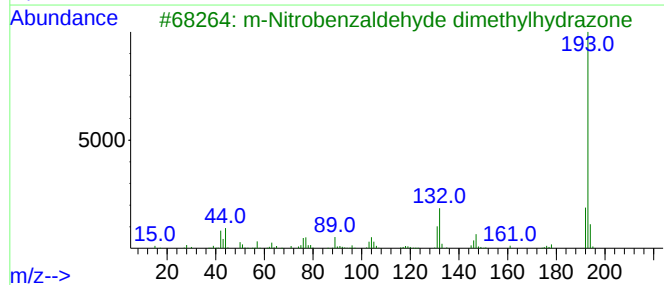
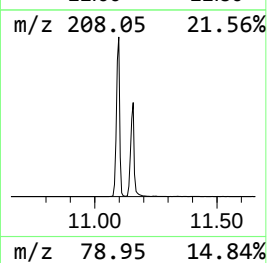
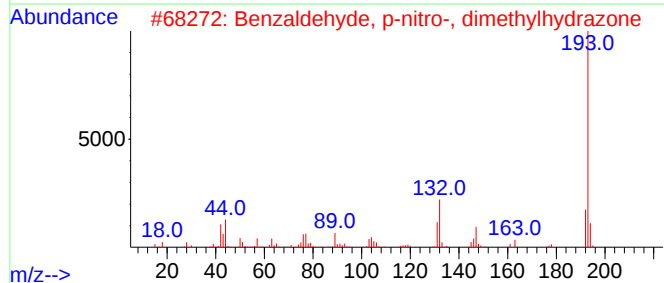
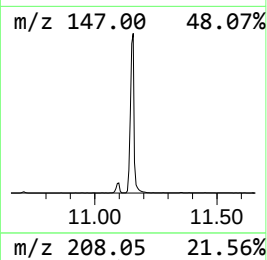
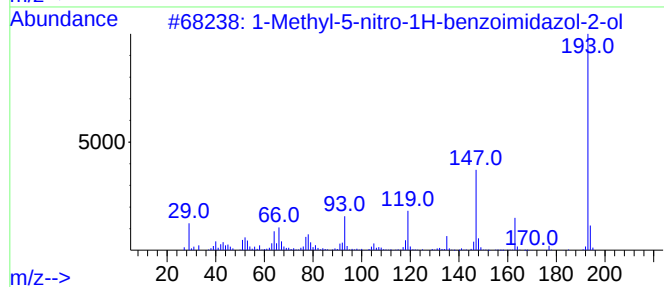
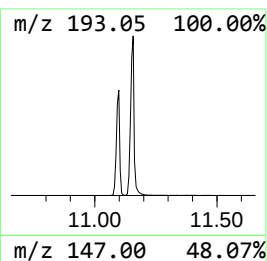
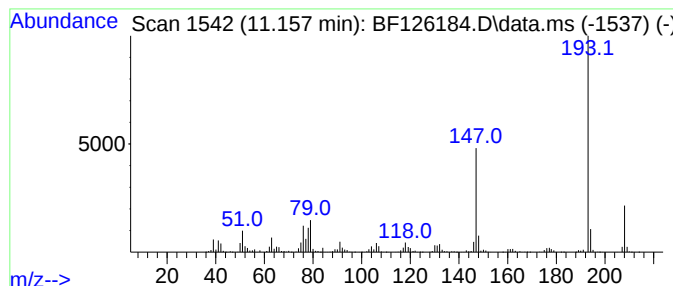
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1-Methyl-5-nitro-1H-benzoim... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.157	56.81 ng	5360550	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-5-nitro-1H-benzoimidazo...	193	C8H7N3O3	066108-85-8	59
2			Benzaldehyde, p-nitro-, dimethyl...	193	C9H11N3O2	010424-92-7	43
3			m-Nitrobenzaldehyde dimethylhydr...	193	C9H11N3O2	032787-76-1	37
4			Benzaldehyde, 2-hydroxy-4-diethy...	208	C11H16N2O2	198280-97-6	35
5			Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
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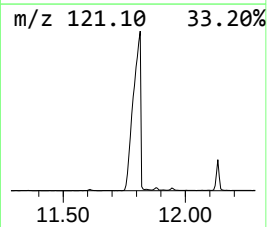
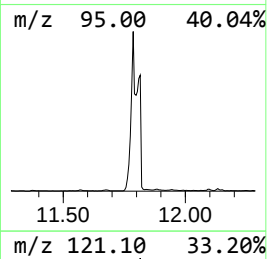
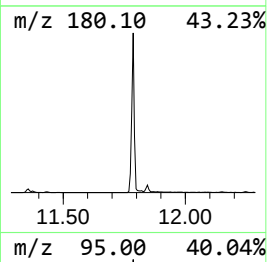
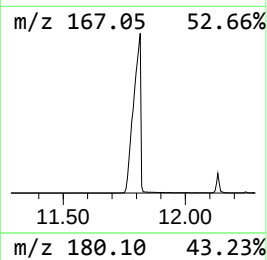
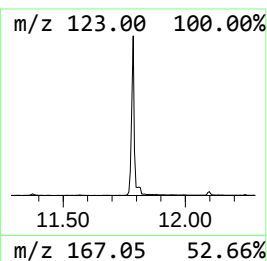
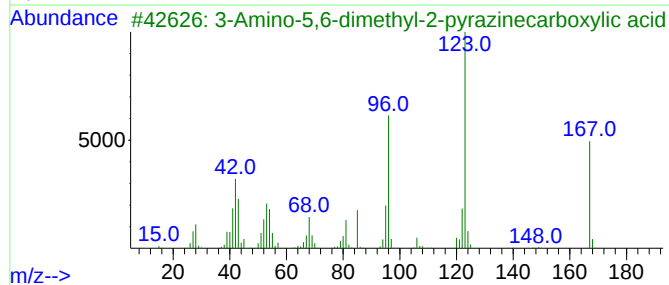
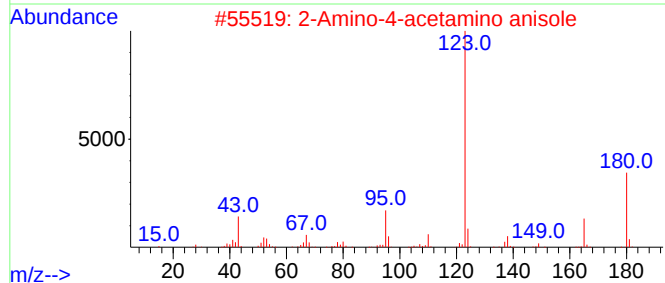
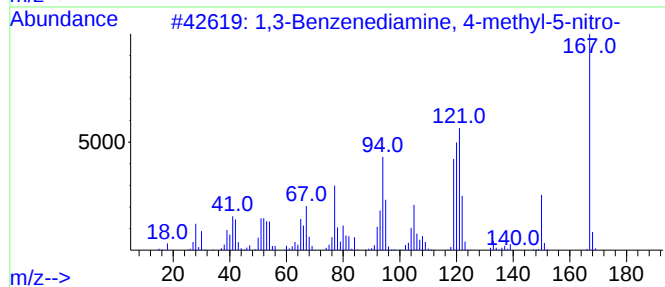
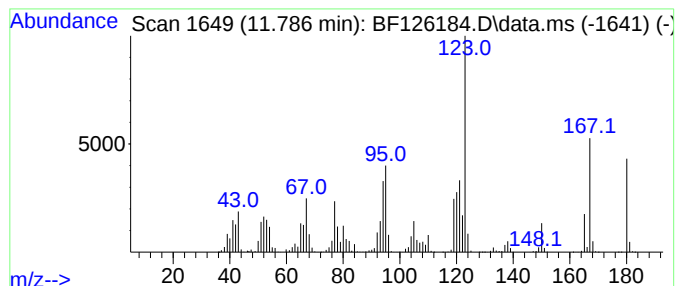
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 2-Amino-4-acetamino anisole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.786	93.50 ng	8822790	Phenanthrene-d10	11.357	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenediamine, 4-methyl-5-n...	167	C7H9N3O2	006629-29-4	94
2	2-Amino-4-acetamino anisole	180	C9H12N2O2	006375-47-9	50
3	3-Amino-5,6-dimethyl-2-pyrazinec...	167	C7H9N3O2	006294-71-9	43
4	Hexahydroindole	123	C8H13N	018159-32-5	41
5	Benzenemethanol, 4-amino-	123	C7H9NO	000623-04-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
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Misc :
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ClientSampleId :
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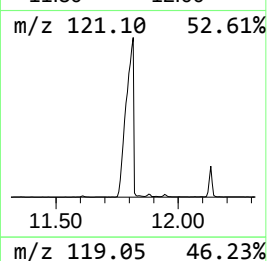
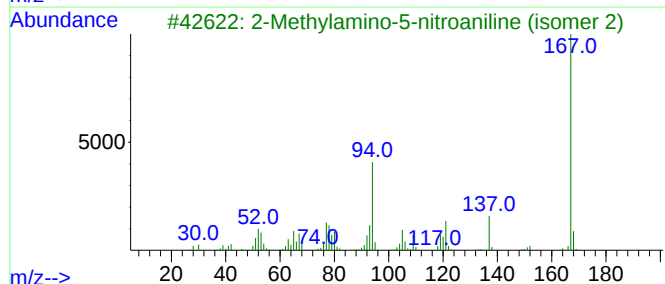
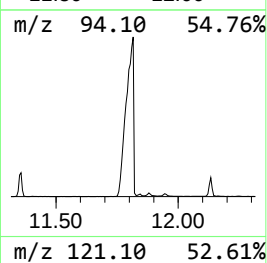
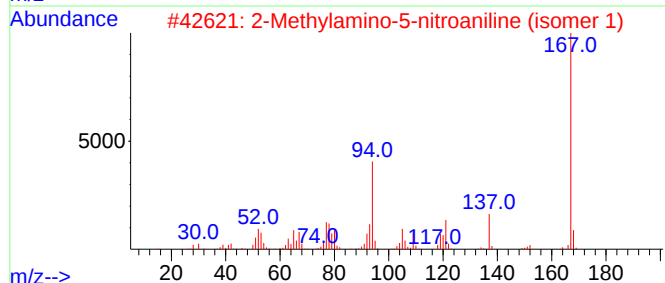
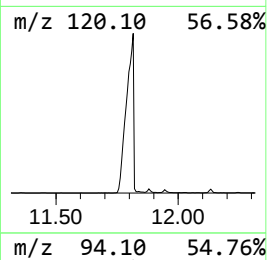
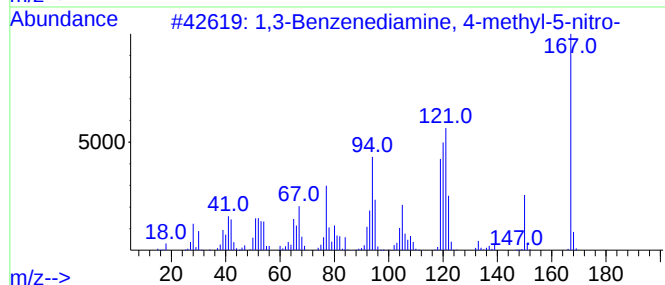
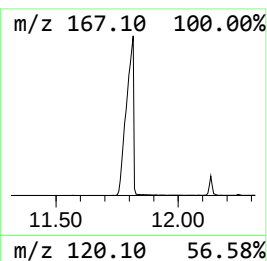
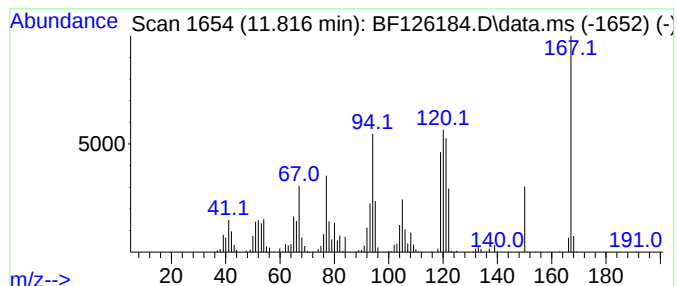
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 1,3-Benzenediamine, 4-methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	59.72 ng	5634670	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenediamine, 4-methyl-5-n...	167	C7H9N3O2	006629-29-4	98
2			2-Methylamino-5-nitroaniline (is...	167	C7H9N3O2	1000477-10-4	43
3			2-Methylamino-5-nitroaniline (is...	167	C7H9N3O2	1000477-10-5	43
4			3-Hydroxy-4-nitrobenzaldehyde	167	C7H5NO4	000704-13-2	43
5			1,3-Benzenediamine, 4-methyl-	122	C7H10N2	000095-80-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
Operator : JU/CG
Sample : M4573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

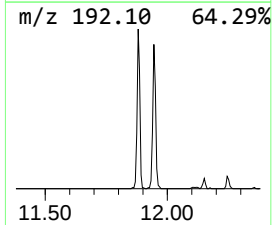
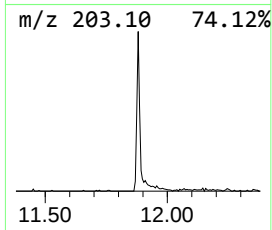
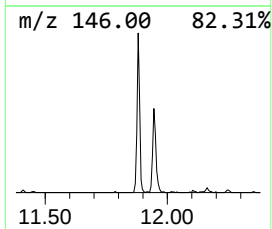
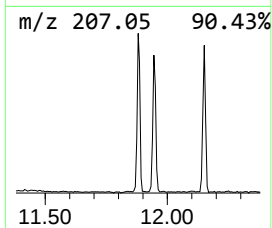
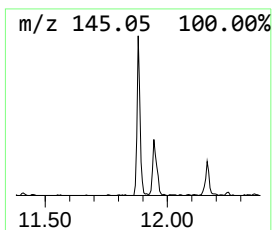
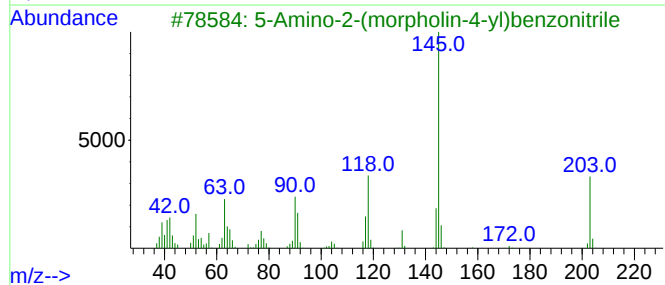
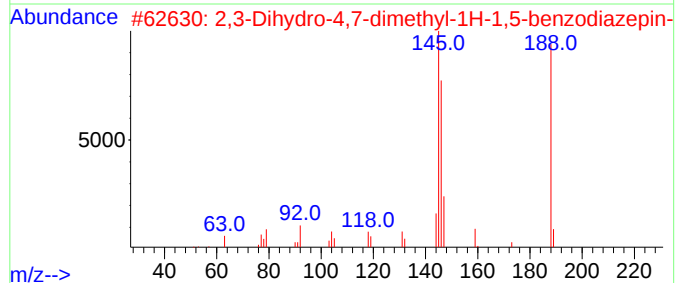
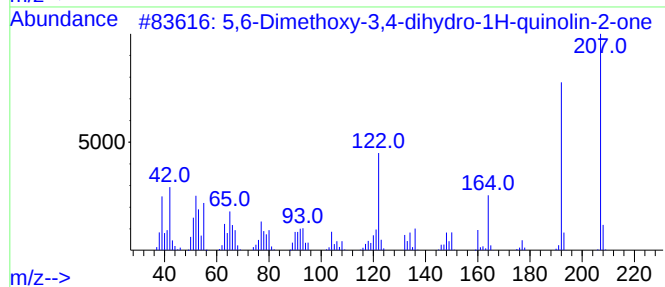
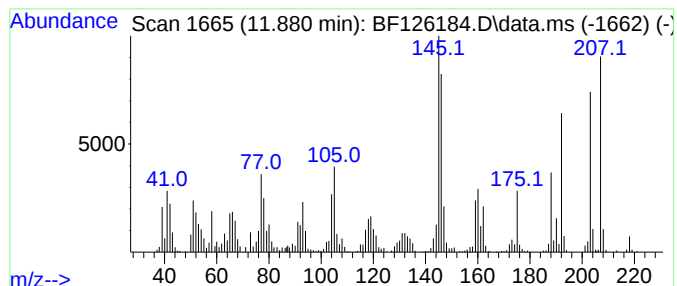
Instrument :
BNA_F
ClientSampleId :
MBR1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown11.880 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.880	14.00 ng	1320580	Phenanthrene-d10	11.357		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,6-Dimethoxy-3,4-dihydro-1H-qui...	207	C11H13NO3	1010434-74-1	47	
2	2,3-Dihydro-4,7-dimethyl-1H-1,5-...	188	C11H12N2O	036743-75-6	42	
3	5-Amino-2-(morpholin-4-yl)benzon...	203	C11H13N3O	078252-12-7	30	
4	1H-Pyrrole, 1-acetyl-2,3-dihydro...	188	C11H12N2O	054966-15-3	30	
5	Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	25	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
Operator : JU/CG
Sample : M4573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MBR1

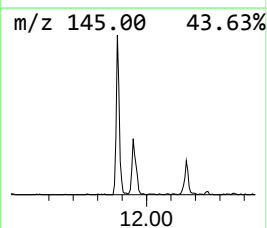
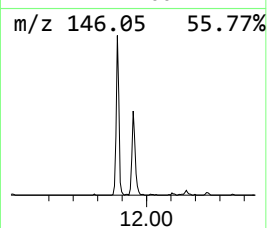
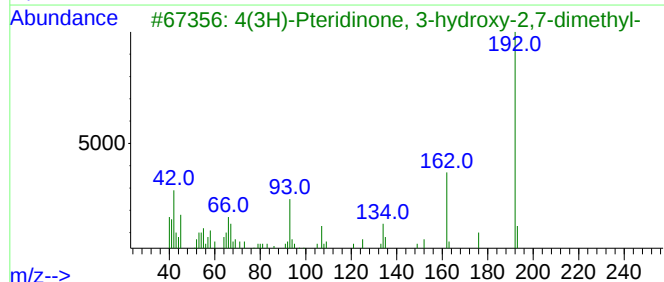
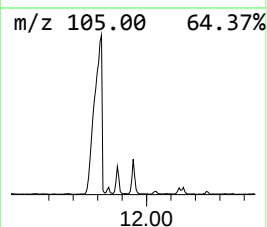
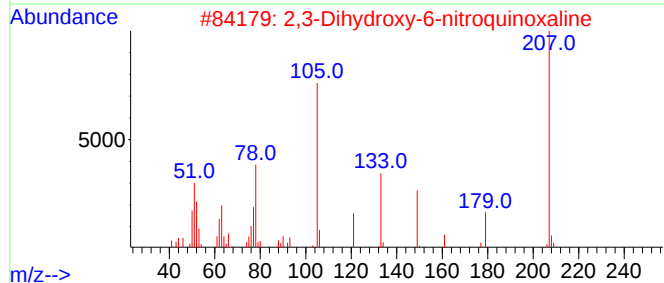
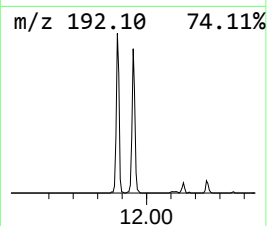
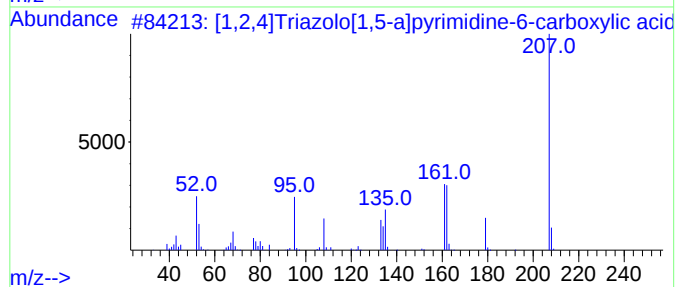
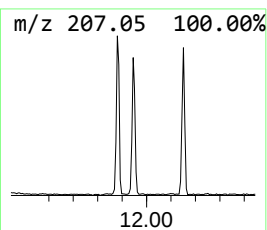
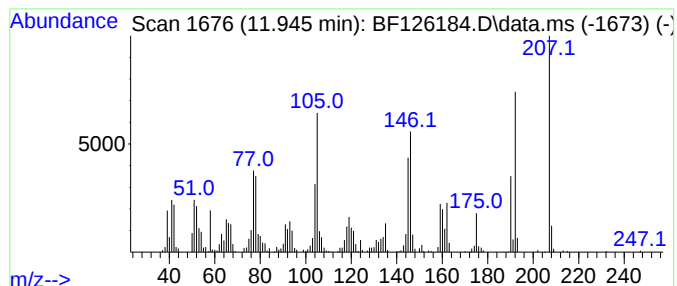
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown11.945 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	10.30 ng	972325	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			[1,2,4]Triazolo[1,5-a]pyrimidine...	207	C8H9N5O2	092673-40-0	41
2			2,3-Dihydroxy-6-nitroquinoxaline	207	C8H5N3O4	002379-56-8	38
3			4(3H)-Pteridinone, 3-hydroxy-2,7...	192	C8H8N4O2	018106-62-2	25
4			1H-1,3-Benzimidazole-2-methanol,...	192	C10H12N2O2	1000351-59-7	20
5			1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126184.D
Acq On : 13 Nov 2021 23:41
Operator : JU/CG
Sample : M4573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MBR1

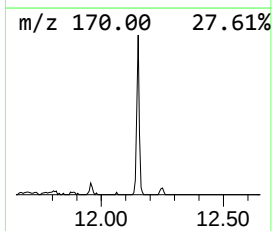
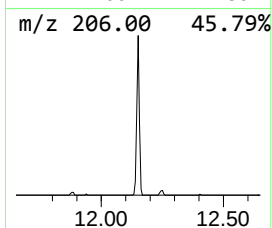
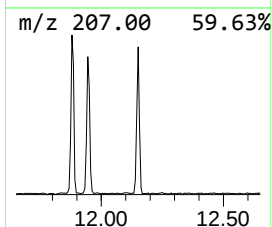
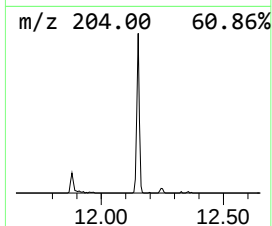
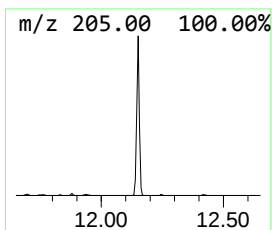
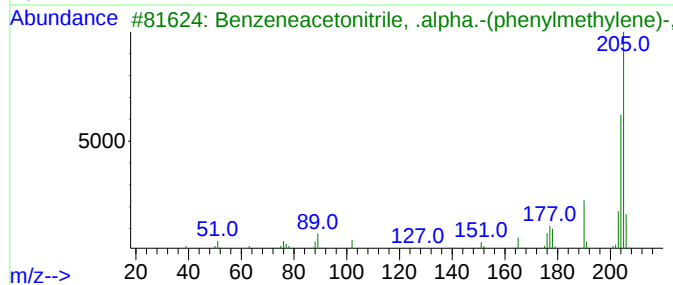
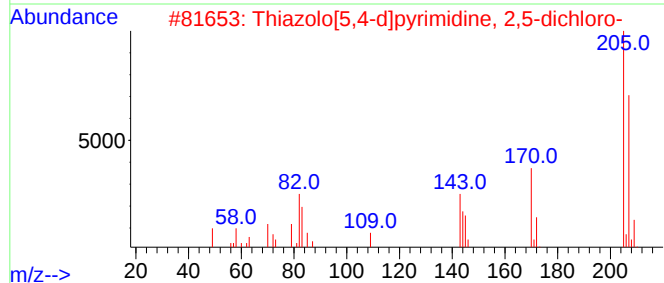
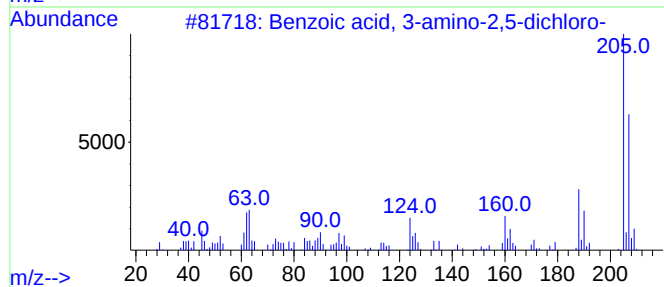
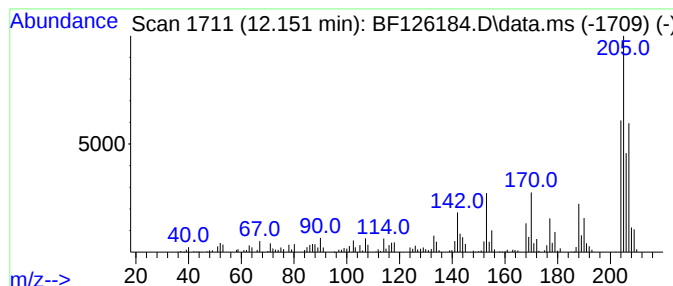
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Benzoic acid, 3-amino-2,5-d... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.151	10.05 ng	948091	Phenanthrene-d10	11.357

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzoic acid, 3-amino-2,5-dichloro-	205	C7H5Cl2NO2	000133-90-4	53
2		Thiazolo[5,4-d]pyrimidine, 2,5-d...	205	C5HC12N3S	013479-89-5	43
3		Benzeneacetonitrile, .alpha.-(ph...	205	C15H11N	016610-80-3	38
4		8-Phenylisoquinoline	205	C15H11N	070125-67-6	38
5		Benzonitrile, 4-(2-phenylethenyl...	205	C15H11N	013041-79-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
 Data File : BF126184.D
 Acq On : 13 Nov 2021 23:41
 Operator : JU/CG
 Sample : M4573-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MBR1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	4.445	26.5	ng	2017160	1	6.828	1522540	20.0
Butanoic acid	4.669	11.3	ng	862742	1	6.828	1522540	20.0
unknown5.634	5.634	36.0	ng	2740700	1	6.828	1522540	20.0
Pentanoic acid	5.892	41.3	ng	3141370	1	6.828	1522540	20.0
Hexanoic acid, ...	7.045	13.5	ng	1030810	1	6.828	1522540	20.0
unknown7.151	7.151	58.6	ng	4463820	1	6.828	1522540	20.0
Phenylethyl Alc...	7.575	14.8	ng	1459430	2	8.116	1966470	20.0
Ethanol, 2-(2-b...	8.028	17.3	ng	1697950	2	8.116	1966470	20.0
Benzeneacetic acid	8.404	19.8	ng	1947010	2	8.116	1966470	20.0
unknown8.822	8.822	9.1	ng	894416	2	8.116	1966470	20.0
1,3-Benzenediam...	9.745	10.1	ng	1163020	3	9.869	2303790	20.0
p-Anisidine, 3-...	10.839	9.7	ng	918489	4	11.357	1887190	20.0
Benzenamine, 2-...	11.051	167.6	ng	15811700	4	11.357	1887190	20.0
unknown11.098	11.098	41.1	ng	3877640	4	11.357	1887190	20.0
1-Methyl-5-nitr...	11.157	56.8	ng	5360550	4	11.357	1887190	20.0
2-Amino-4-aceta...	11.786	93.5	ng	8822790	4	11.357	1887190	20.0
1,3-Benzenediam...	11.816	59.7	ng	5634670	4	11.357	1887190	20.0
unknown11.880	11.880	14.0	ng	1320580	4	11.357	1887190	20.0
unknown11.945	11.945	10.3	ng	972325	4	11.357	1887190	20.0
Benzoic acid, 3...	12.151	10.1	ng	948091	4	11.357	1887190	20.0