

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
 Data File : BG051053.D
 Acq On : 15 Nov 2021 22:49
 Operator : CG/JU
 Sample : M4573-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 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_G\Methods\8270-BG111321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051053.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.034	75	93	102	rVB	128695	458440	4.97%	1.070%
2	4.322	130	142	155	rVB	78901	212694	2.30%	0.496%
3	5.245	256	299	302	rBV	241416	1805906	19.56%	4.214%
4	5.409	302	327	331	rVB2	205818	990176	10.73%	2.311%
5	5.762	373	387	391	rBV	244412	608885	6.60%	1.421%
6	6.091	437	443	452	rVB2	54068	95814	1.04%	0.224%
7	7.236	629	638	648	rBV2	55054	124633	1.35%	0.291%
8	7.372	654	661	673	rVB	108968	201347	2.18%	0.470%
9	8.223	799	806	811	rBV	135588	254376	2.76%	0.594%
10	8.282	811	816	831	rVV3	62315	217582	2.36%	0.508%
11	8.523	835	857	873	rVV2	233558	986131	10.68%	2.301%
12	8.858	902	914	920	rBV	121571	294218	3.19%	0.687%
13	9.399	998	1006	1015	rBV	402363	719645	7.79%	1.679%
14	9.780	1063	1071	1088	rBV	132764	332433	3.60%	0.776%
15	10.350	1163	1168	1176	rVB3	49534	95098	1.03%	0.222%
16	10.797	1239	1244	1261	rVB	170759	316338	3.43%	0.738%
17	11.050	1279	1287	1297	rVB	199533	358931	3.89%	0.838%
18	11.420	1341	1350	1368	rBV3	84009	179787	1.95%	0.420%
19	11.631	1371	1386	1396	rBV	278475	764550	8.28%	1.784%
20	12.659	1552	1561	1588	rBV2	98565	441115	4.78%	1.029%
21	13.470	1691	1699	1706	rBV	1008581	1574966	17.06%	3.675%
22	14.616	1887	1894	1898	rBV	282712	497903	5.39%	1.162%
23	14.657	1898	1901	1912	rVB2	82700	148951	1.61%	0.348%
24	14.851	1925	1934	1943	rVB	343852	549875	5.96%	1.283%
25	15.785	2084	2093	2102	rBV2	55538	110290	1.19%	0.257%
26	15.920	2108	2116	2124	rBV	143456	235465	2.55%	0.549%
27	16.337	2181	2187	2195	rVV	515798	796720	8.63%	1.859%
28	16.420	2195	2201	2207	rVV	120238	189679	2.05%	0.443%
29	16.661	2234	2242	2252	rBV2	178255	318750	3.45%	0.744%
30	17.031	2288	2305	2311	rBV	3109719	6302366	68.26%	14.707%
31	17.107	2311	2318	2328	rVB	1091709	1659462	17.97%	3.872%
32	17.213	2328	2336	2350	rBV	1662114	2727031	29.54%	6.364%
33	17.601	2395	2402	2412	rBV	411830	644923	6.99%	1.505%
34	18.300	2513	2521	2523	rBV	959027	1522831	16.49%	3.554%
35	18.365	2523	2532	2537	rVV	3754579	9232288	100.00%	21.544%
36	18.453	2539	2547	2550	rVV2	213723	404019	4.38%	0.943%

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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_G\Methods\8270-BG111321.M
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37	18.488	2550	2553	2564	rVV	212814	352412	3.82%	0.822%
38	18.600	2566	2572	2579	rVB2	265838	443357	4.80%	1.035%
39	18.929	2622	2628	2631	rBV	229641	355292	3.85%	0.829%
40	18.964	2631	2634	2640	rVB2	211337	318897	3.45%	0.744%
41	19.105	2649	2658	2665	rVB	395035	575218	6.23%	1.342%
42	19.269	2678	2686	2690	rBV2	127460	177425	1.92%	0.414%
43	19.387	2702	2706	2711	rVB3	74367	92972	1.01%	0.217%
44	20.186	2836	2842	2851	rBV	1768293	2389783	25.89%	5.577%
45	20.533	2897	2901	2911	rVV3	90918	168250	1.82%	0.393%
46	21.484	3059	3063	3075	rVB2	105512	227728	2.47%	0.531%
47	21.896	3127	3133	3141	rVB	364821	633775	6.86%	1.479%
48	23.400	3385	3389	3398	rVB2	61147	118587	1.28%	0.277%
49	25.303	3703	3713	3725	rVB2	194613	625659	6.78%	1.460%

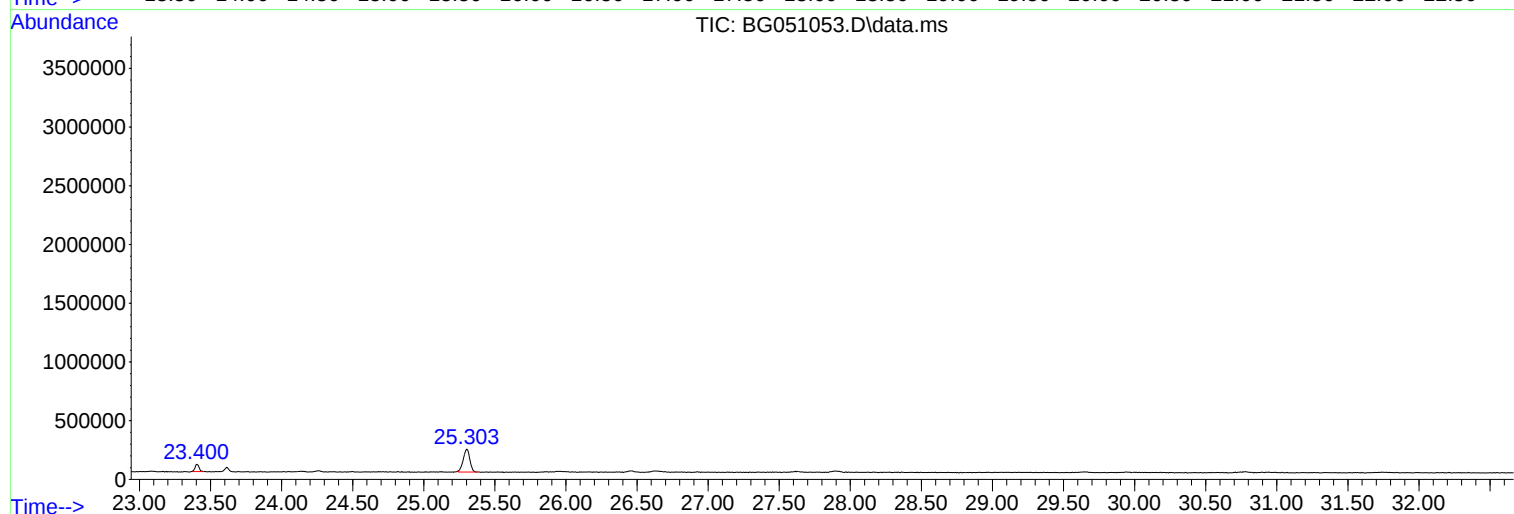
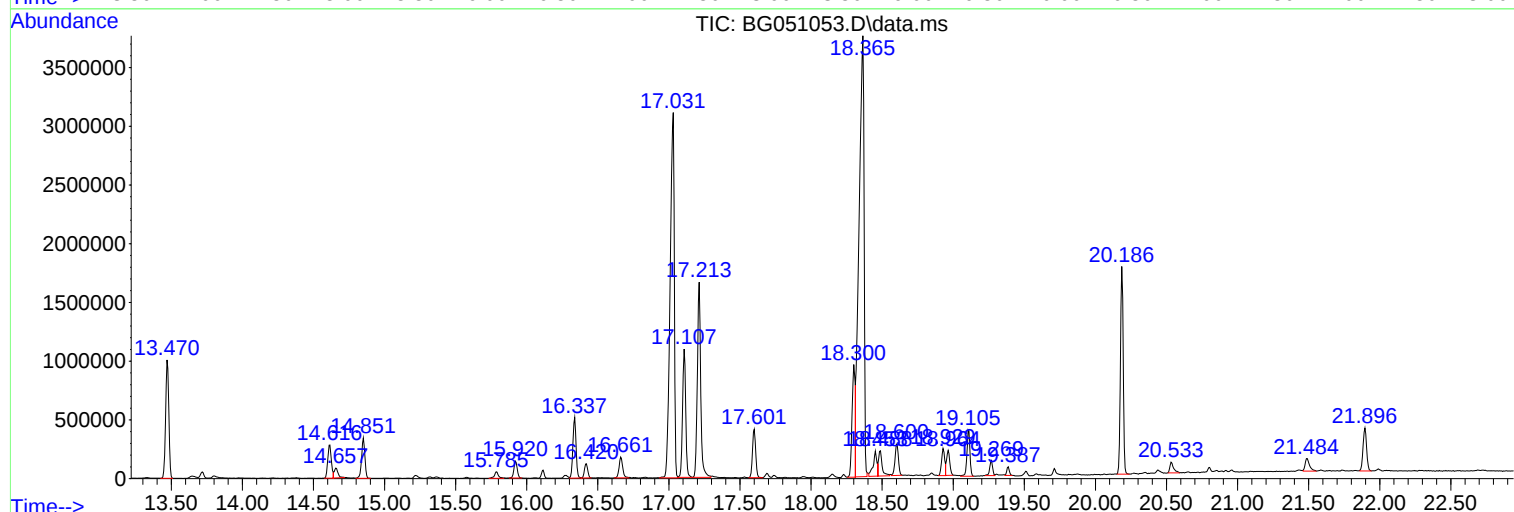
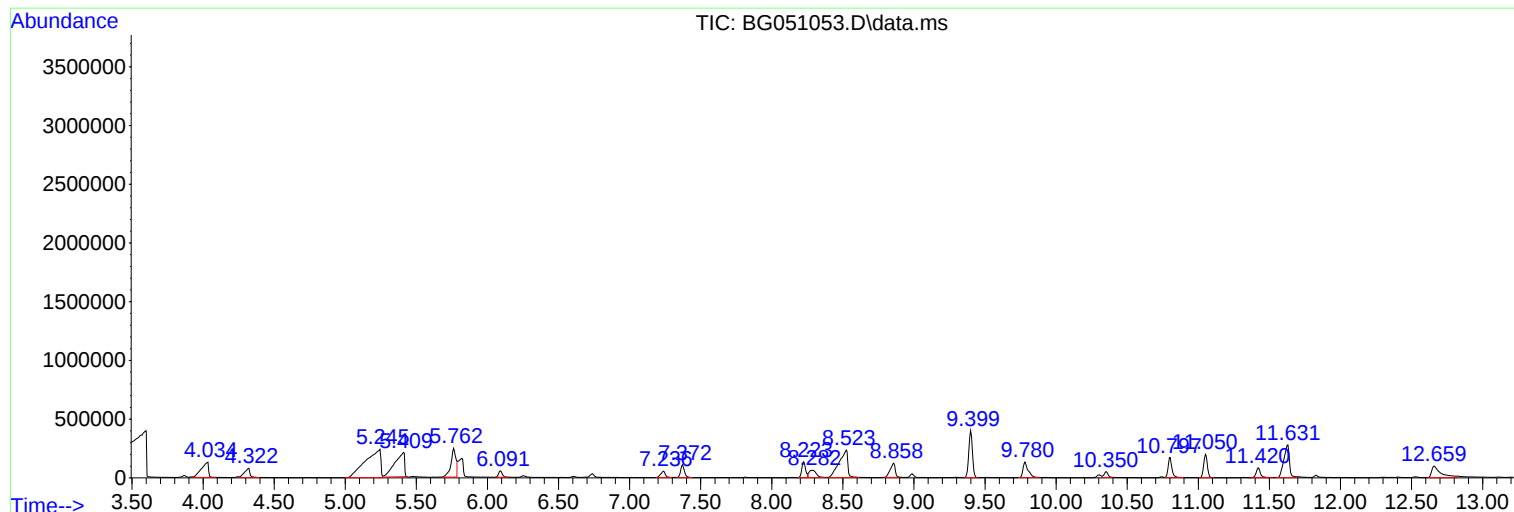
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ClientSampleId :
MBR1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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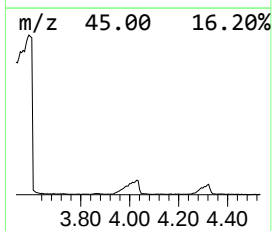
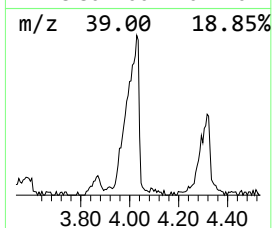
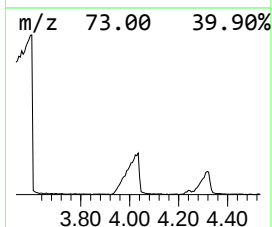
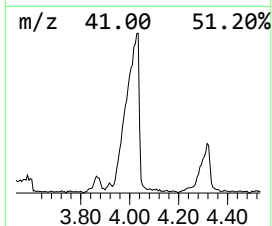
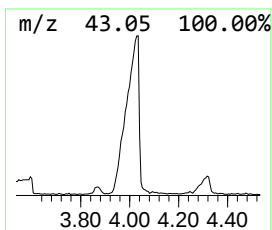
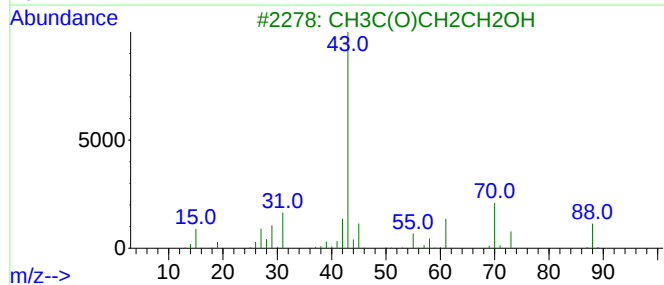
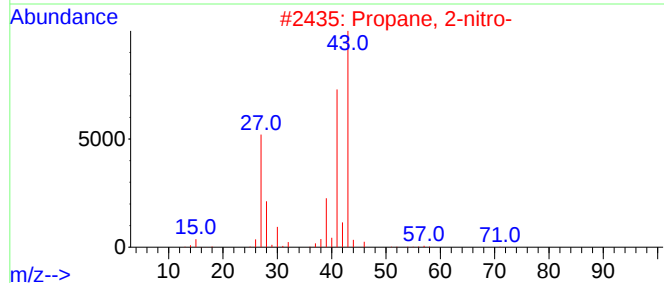
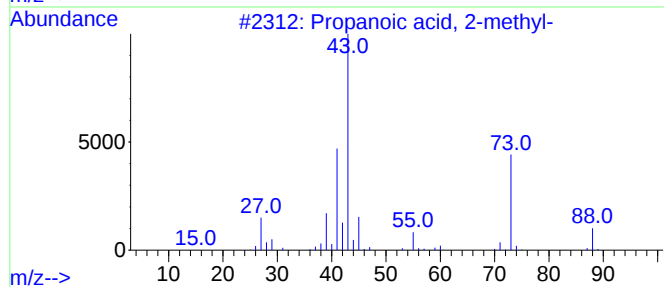
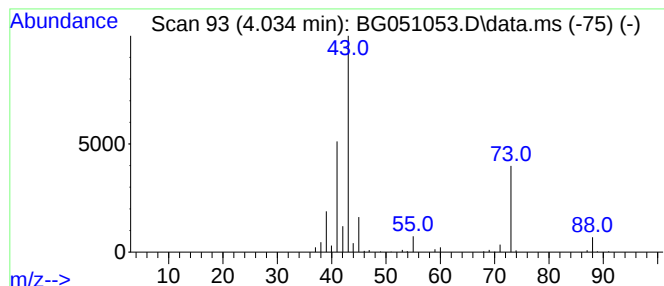
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.034	36.04 ng	458440	1,4-Dichlorobenzene-d4	8.223

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	91
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	12
3			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	9
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	9



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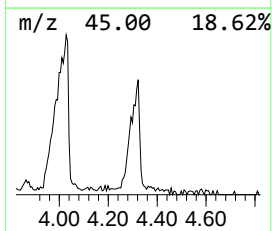
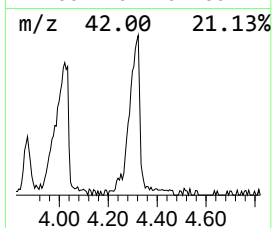
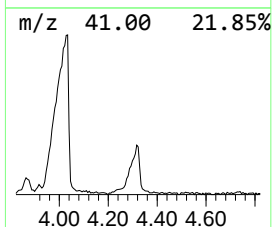
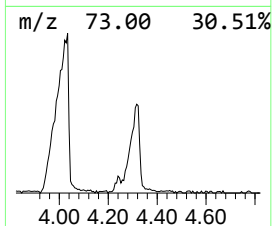
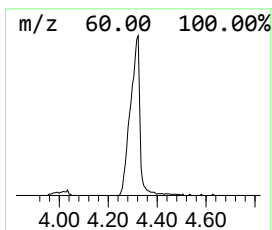
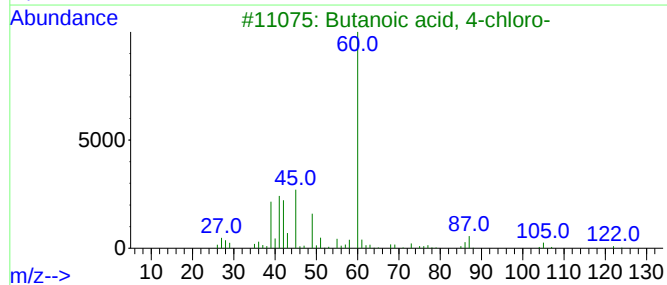
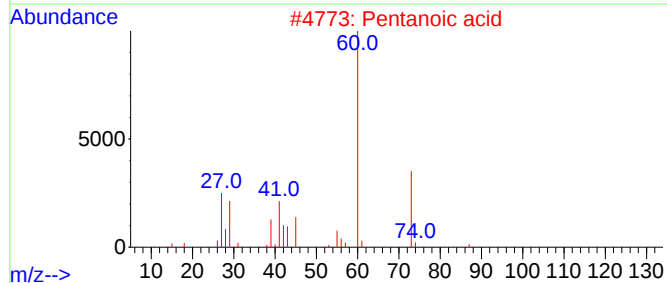
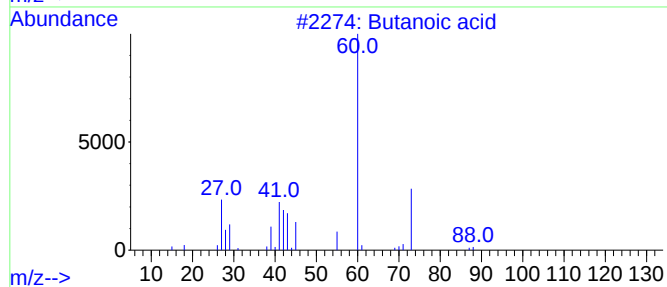
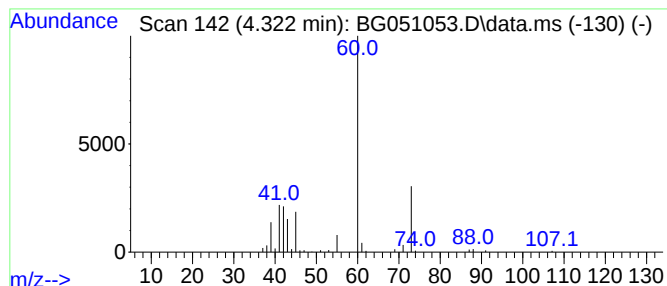
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.322	16.72 ng	212694	1,4-Dichlorobenzene-d4	8.223

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	91
2			Pentanoic acid	102	C5H10O2	000109-52-4	50
3			Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	39
4			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	9
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	9



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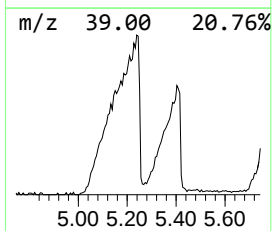
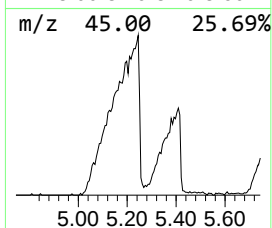
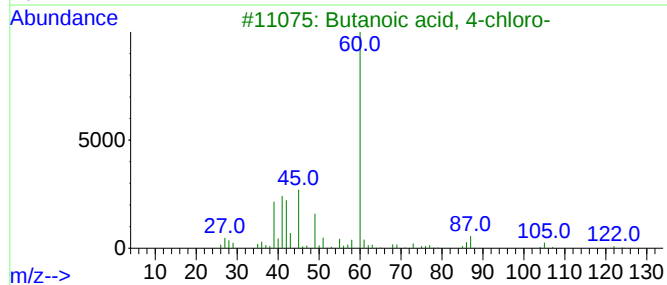
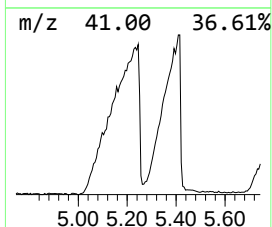
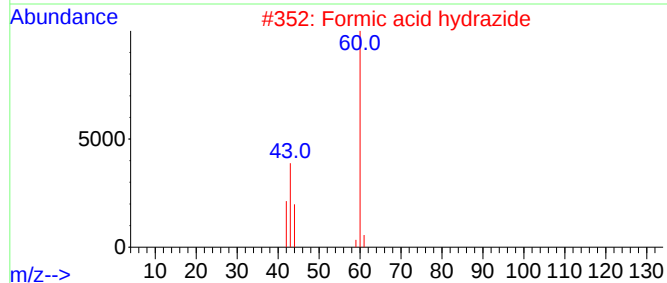
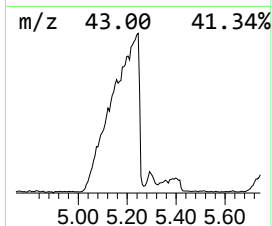
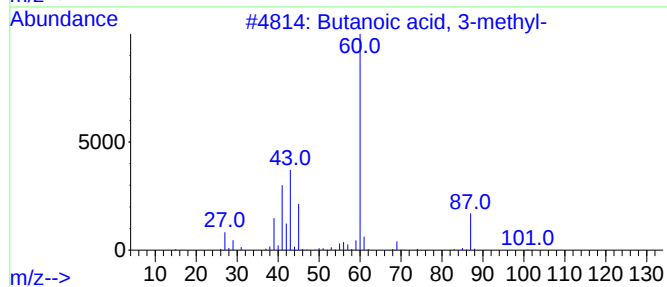
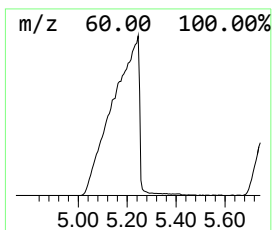
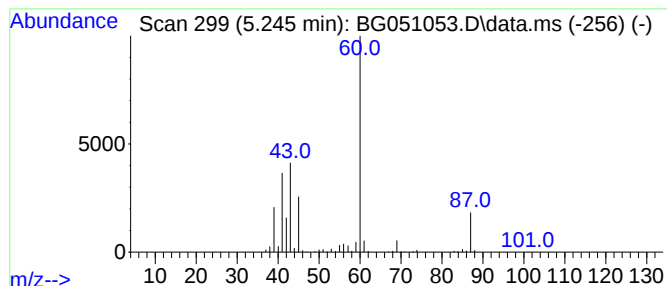
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.245	141.99 ng	1805910	1,4-Dichlorobenzene-d4	8.223

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	90
2			Formic acid hydrazide	60	CH4N2O	000624-84-0	50
3			Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	39
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	39
5			Pentanoic acid	102	C5H10O2	000109-52-4	38



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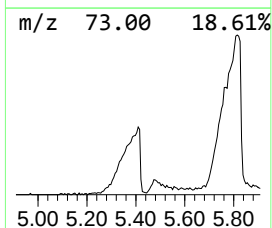
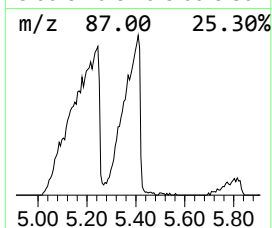
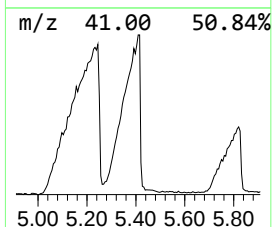
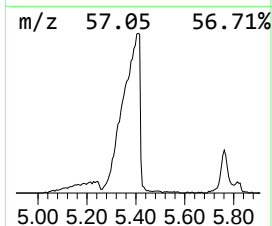
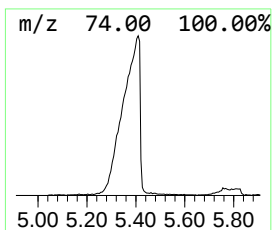
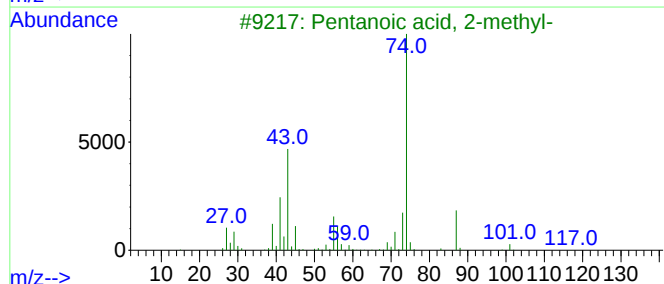
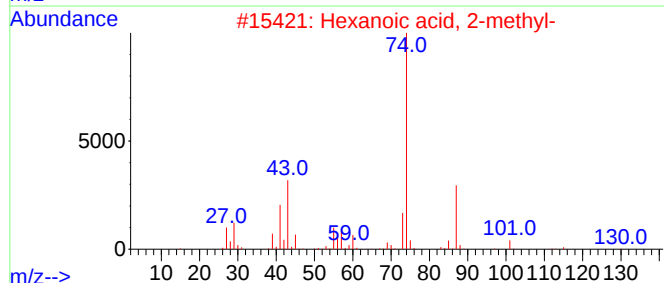
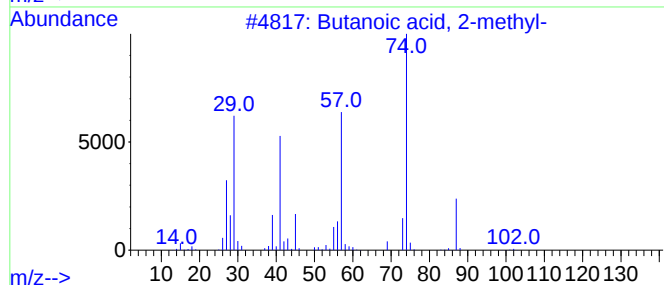
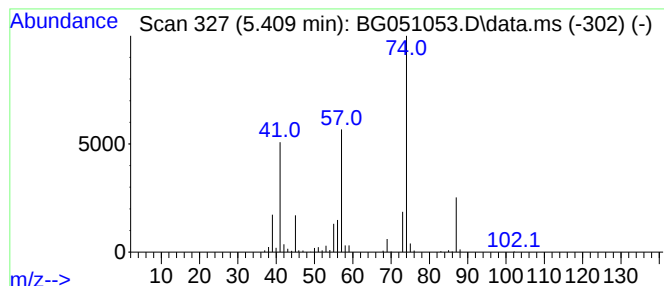
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Pentanoic acid, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.409	77.85 ng	990176	1,4-Dichlorobenzene-d4	8.223

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	91
2			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	64
3			Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	64
4			Methyl valerate	116	C6H12O2	000624-24-8	40
5			2,4-Dimethylpentanoic acid	130	C7H14O2	005868-33-7	40



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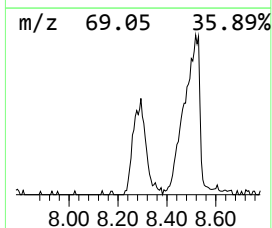
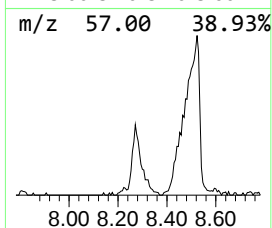
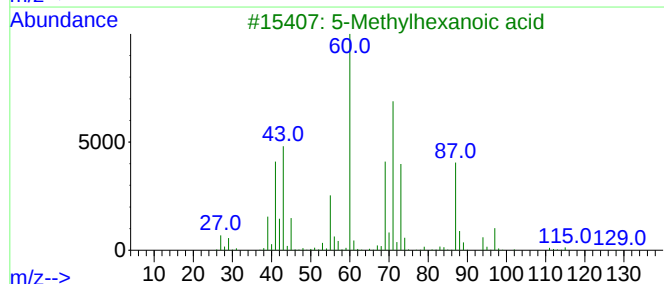
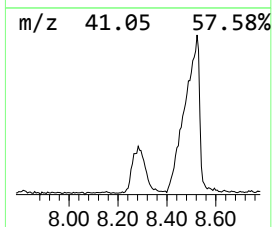
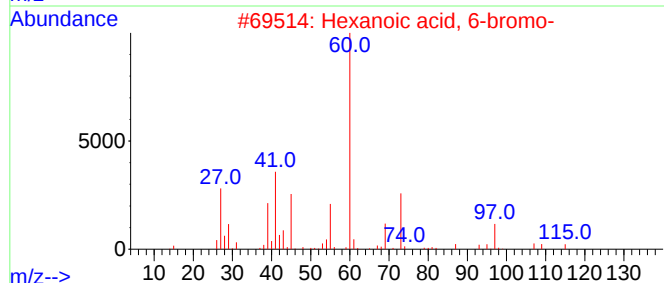
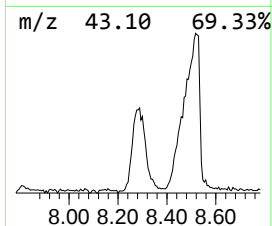
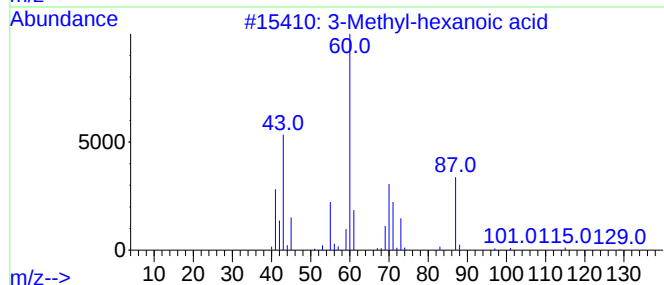
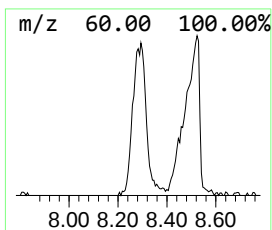
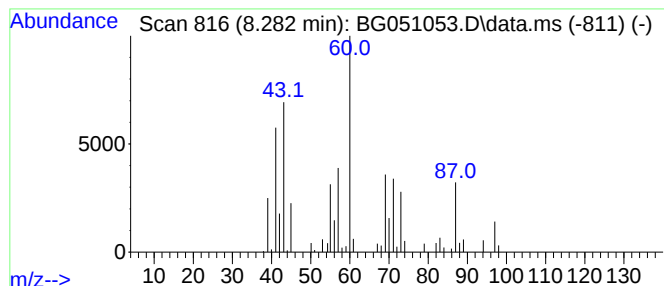
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 3-Methyl-hexanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.282	17.11 ng	217582	1,4-Dichlorobenzene-d4	8.223

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	50
2			Hexanoic acid, 6-bromo-	194	C6H11BrO2	004224-70-8	50
3			5-Methylhexanoic acid	130	C7H14O2	000628-46-6	47
4			.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	43
5			Phospholane	88	C4H9P	003466-00-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
Operator : CG/JU
Sample : M4573-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MBR1

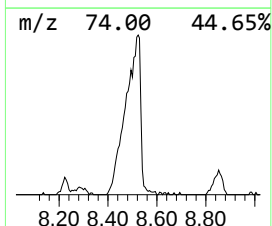
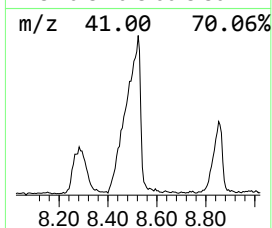
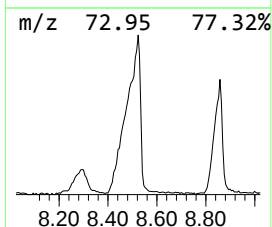
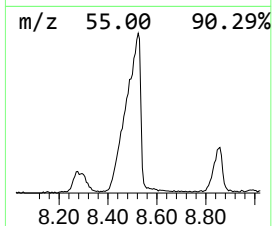
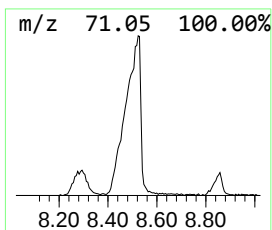
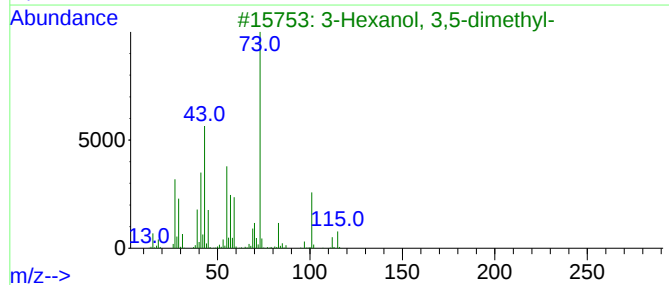
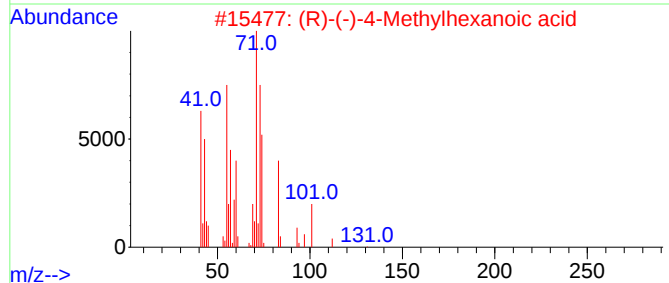
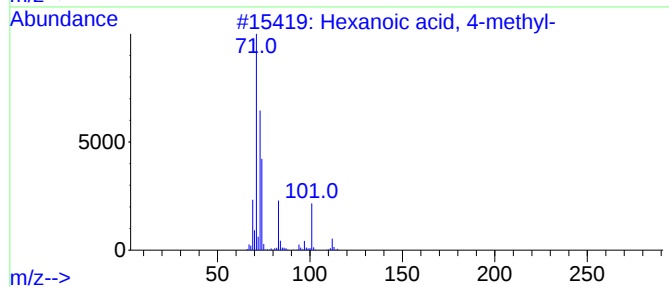
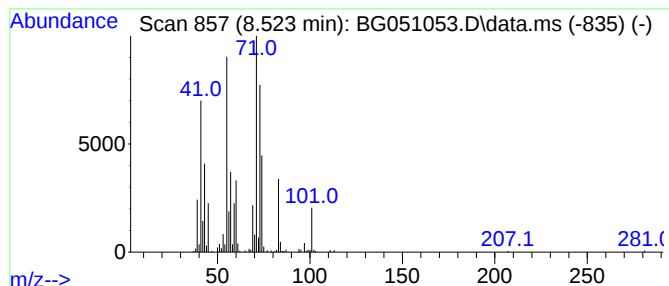
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexanoic acid, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.523	77.53 ng	986131	1,4-Dichlorobenzene-d4	8.223

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 4-methyl-	130	C7H14O2	001561-11-1	74
2			(R)-(-)-4-Methylhexanoic acid	130	C7H14O2	052745-93-4	50
3			3-Hexanol, 3,5-dimethyl-	130	C8H18O	004209-91-0	14
4			Oxirane, 3-hydroxypropyl-	102	C5H10O2	021915-56-0	14
5			4-Nonanol	144	C9H20O	005932-79-6	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
Operator : CG/JU
Sample : M4573-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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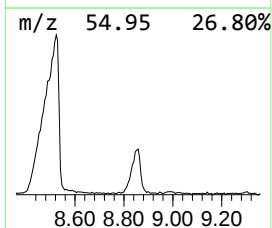
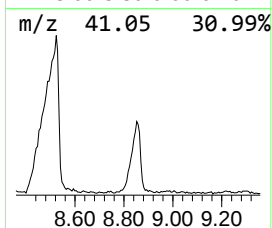
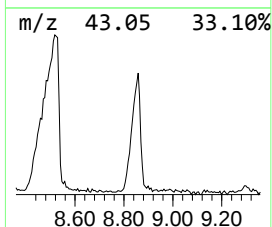
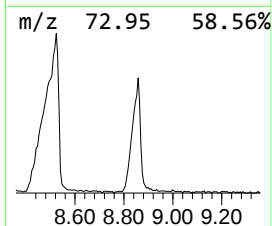
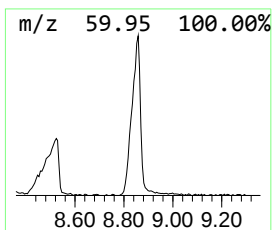
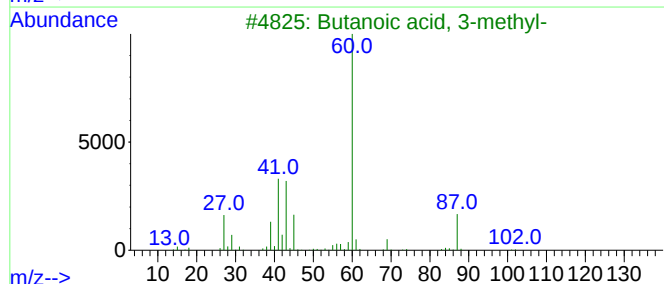
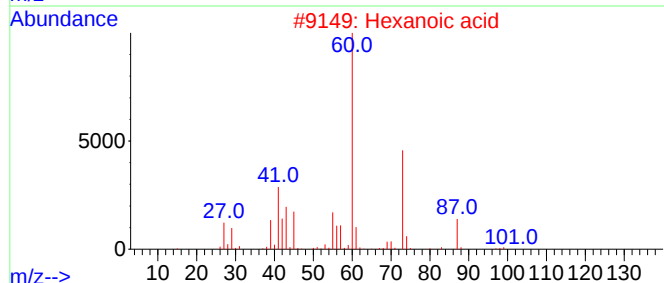
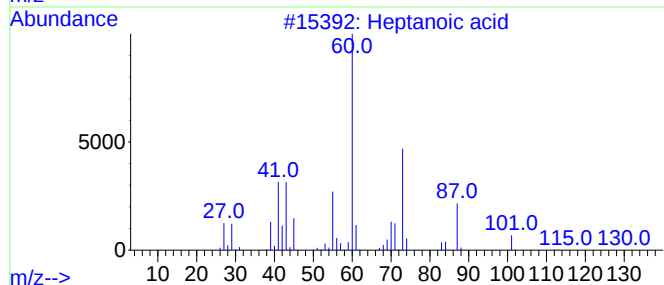
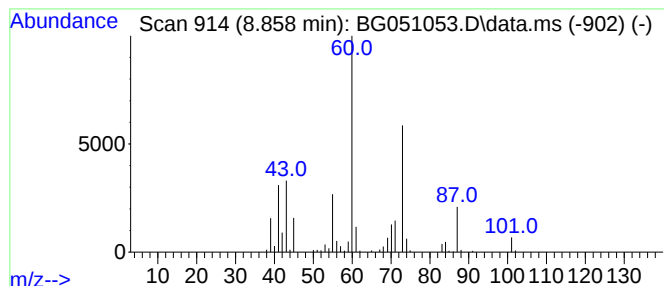
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.858	23.13 ng	294218	1,4-Dichlorobenzene-d4	8.223

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanoic acid	130	C7H14O2	000111-14-8	90
2			Hexanoic acid	116	C6H12O2	000142-62-1	64
3			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
4			Pentanoic acid	102	C5H10O2	000109-52-4	53
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
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Sample : M4573-01
Misc :
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ClientSampleId :
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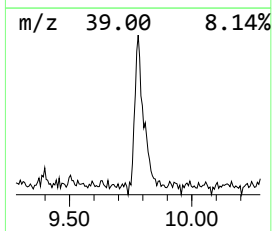
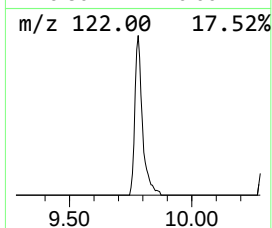
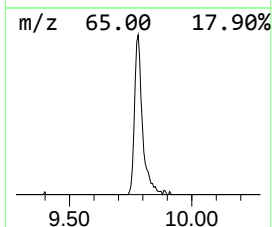
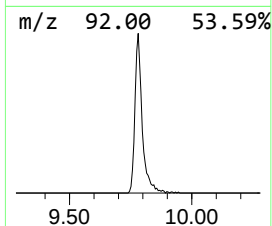
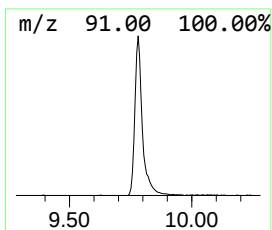
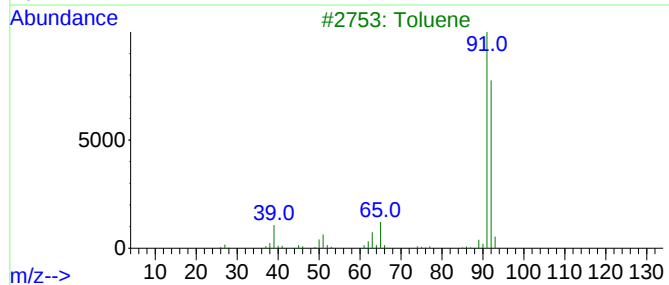
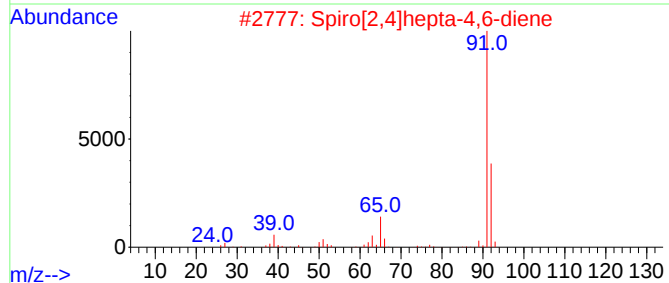
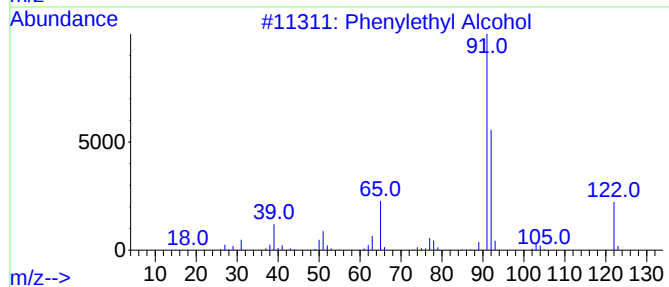
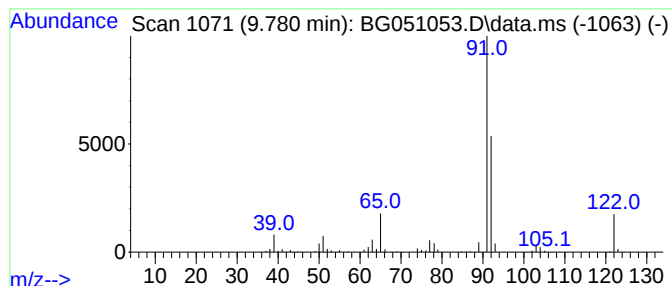
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenylethyl Alcohol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.780	18.52 ng	332433	Naphthalene-d8	11.050

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			Toluene	92	C7H8	000108-88-3	76
4			Tetracyclo[3.2.0.0(2,7).0(4,6)]h...	92	C7H8	000278-06-8	64
5			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
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Acq On : 15 Nov 2021 22:49
Operator : CG/JU
Sample : M4573-01
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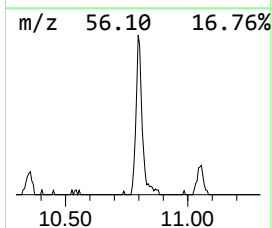
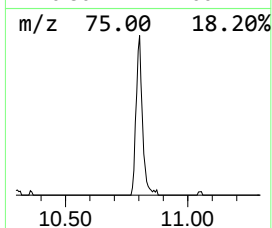
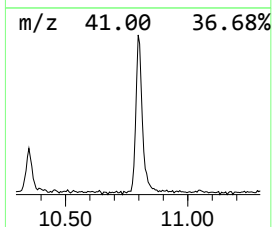
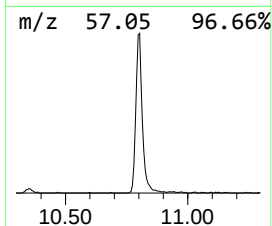
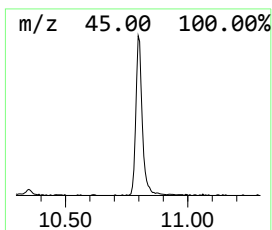
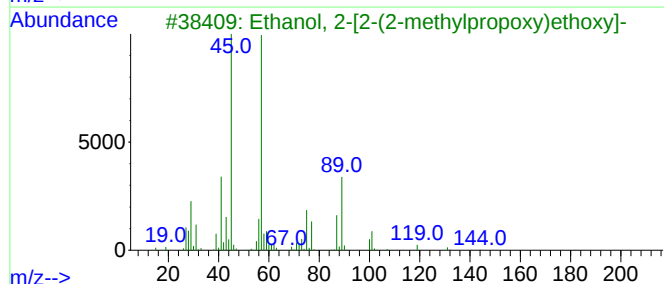
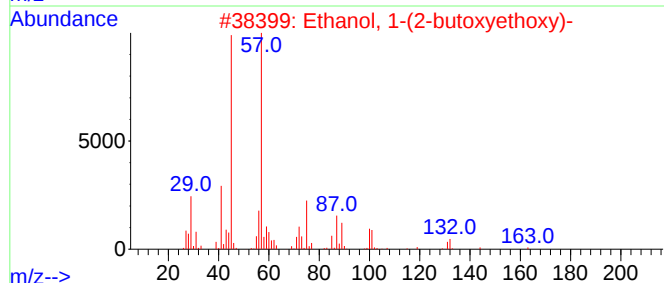
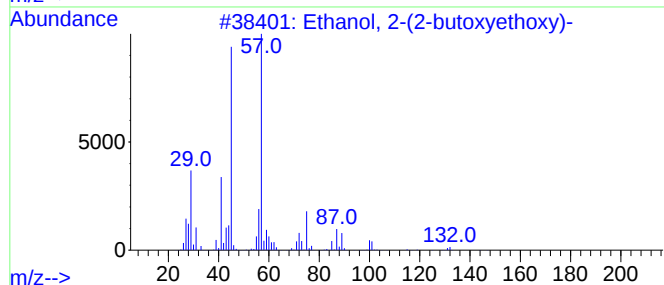
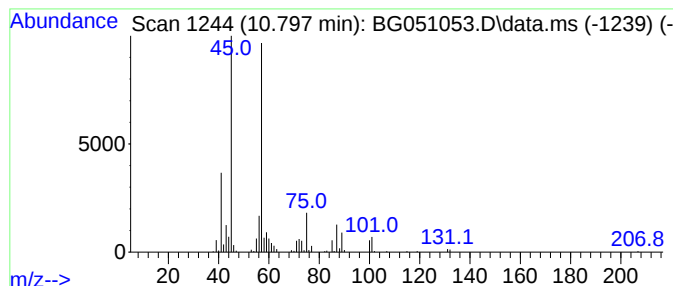
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.797	17.63 ng	316338	Naphthalene-d8	11.050	
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	86
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
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Instrument :
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ClientSampleId :
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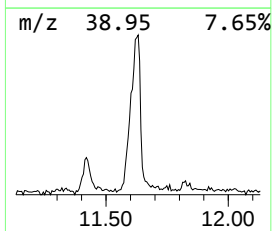
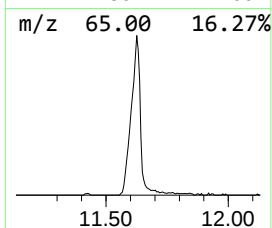
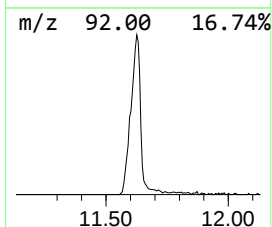
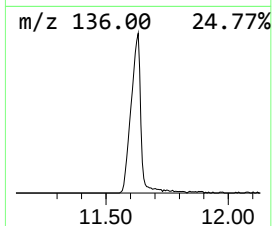
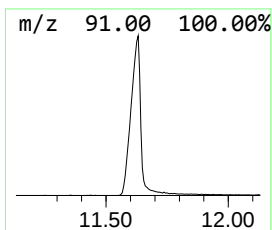
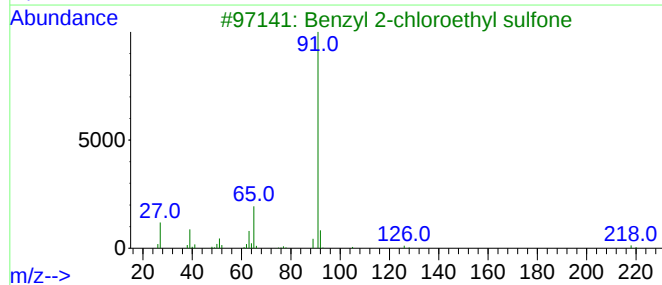
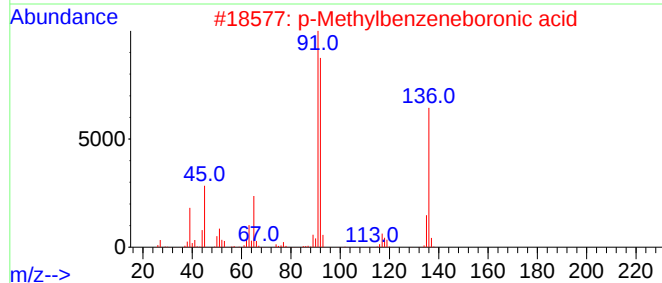
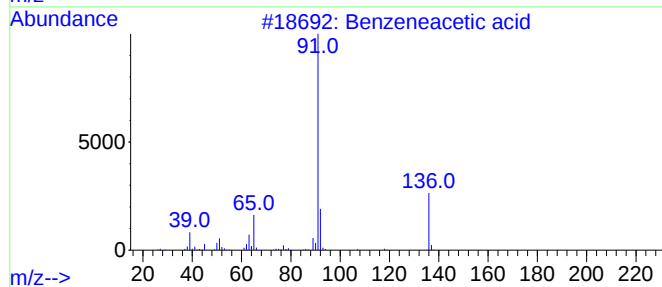
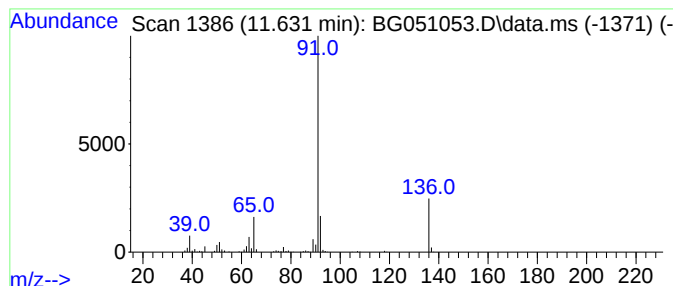
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzeneacetic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.631	42.60 ng	764550	Naphthalene-d8	11.050

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	95
2			p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	64
3			Benzyl 2-chloroethyl sulfone	218	C9H11ClO2S	066998-67-2	50
4			12-Benzyl-4,9,15-trioxa-3,5,8,10...	325	C13H7N7O4	1394125-25-7	50
5			Toluene	92	C7H8	000108-88-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
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Misc :
ALS Vial : 13 Sample Multiplier: 1

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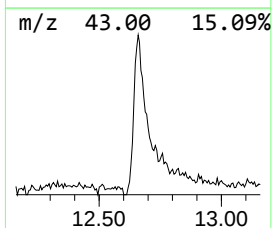
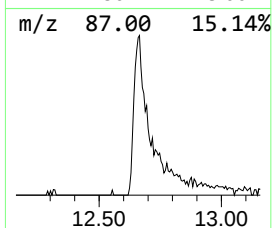
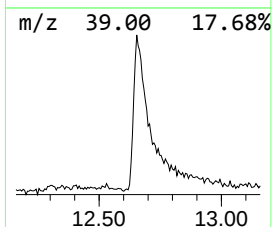
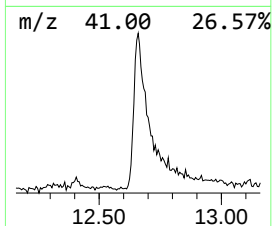
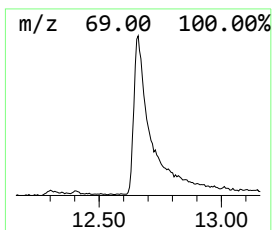
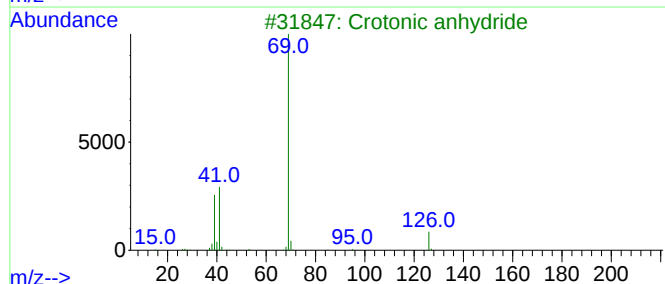
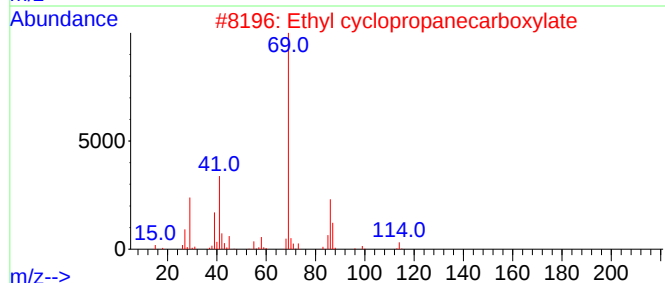
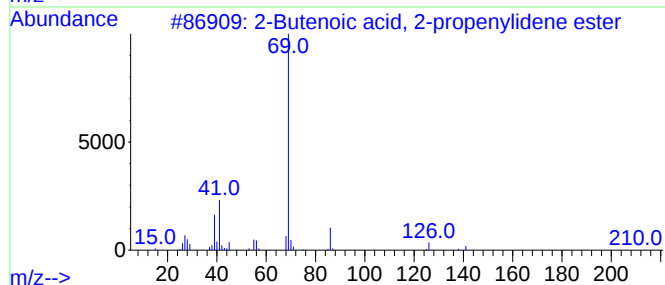
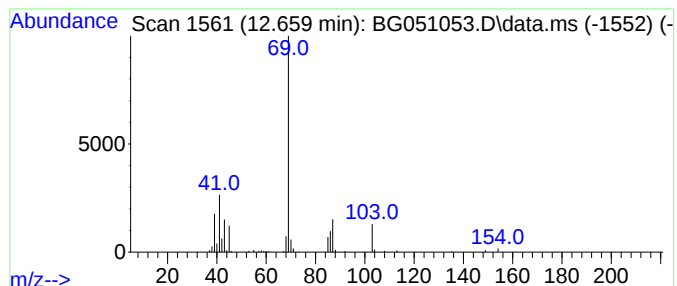
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown12.659 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.659	24.58 ng	441115	Naphthalene-d8	11.050

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
2		Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38
3		Crotonic anhydride	154	C8H10O3	000623-68-7	28
4		Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	9
5		Oxazole	69	C3H3NO	000288-42-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
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Sample : M4573-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

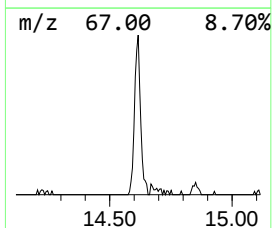
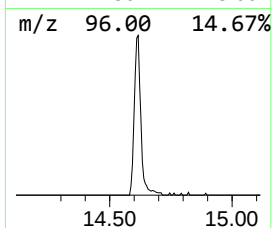
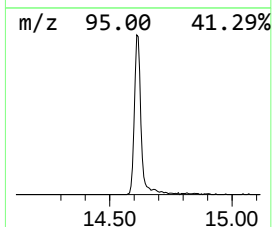
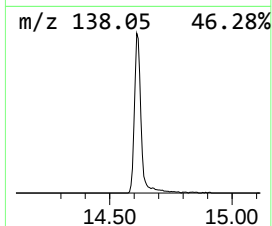
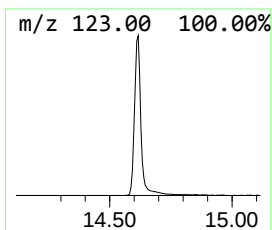
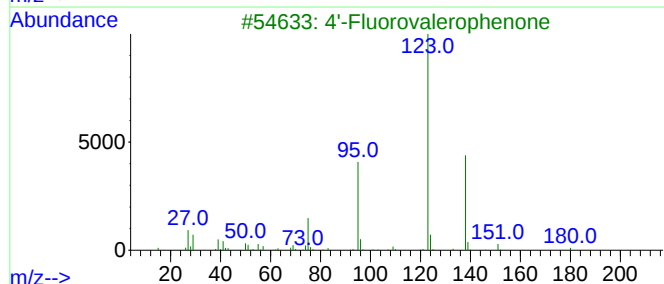
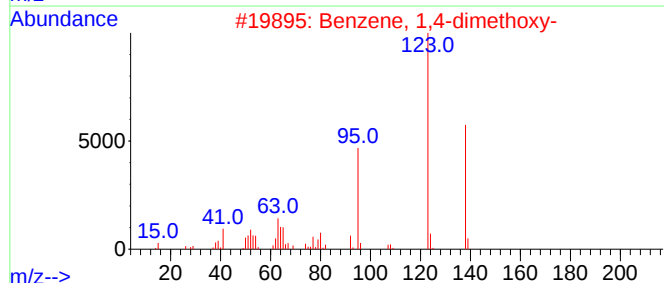
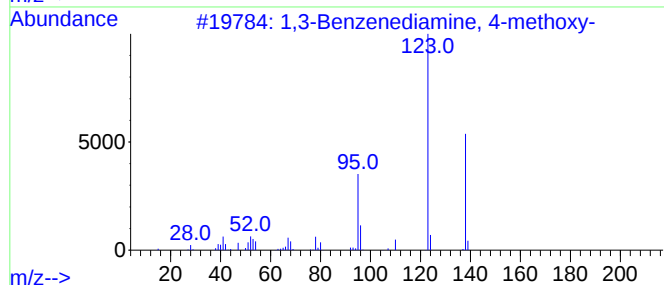
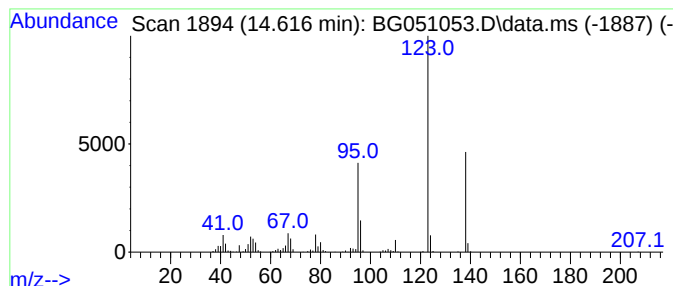
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ClientSampleId :
MBR1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,3-Benzenediamine, 4-methoxy- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.616	18.11 ng	497903	Acenaphthene-d10			14.851
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,3-Benzenediamine, 4-methoxy-		138	C7H10N2O	000615-05-4	97
2	Benzene, 1,4-dimethoxy-		138	C8H10O2	000150-78-7	87
3	4'-Fluorovalerophenone		180	C11H13FO	029114-66-7	78
4	2-Methoxy-5-methylphenol		138	C8H10O2	001195-09-1	72
5	1,3-Benzenediol, 4-ethyl-		138	C8H10O2	002896-60-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
Operator : CG/JU
Sample : M4573-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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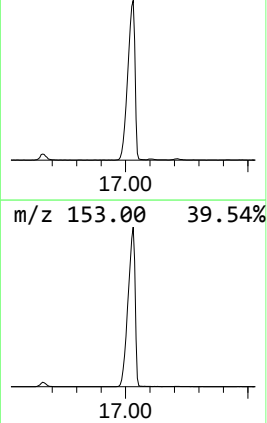
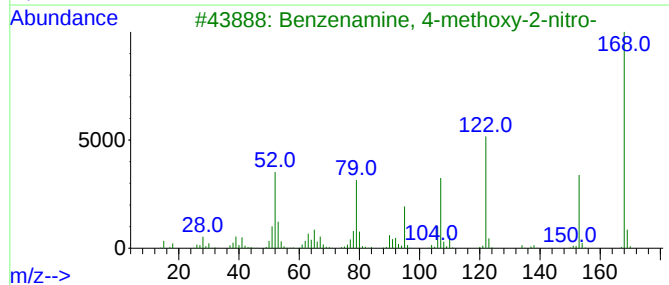
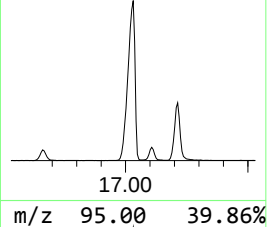
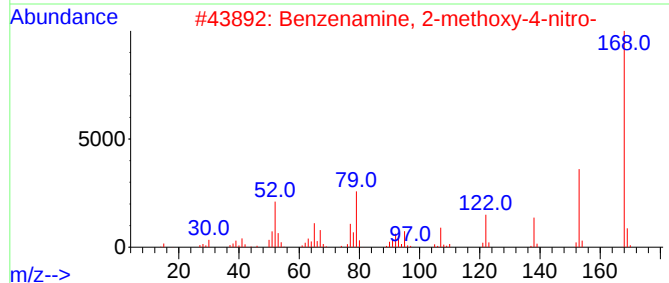
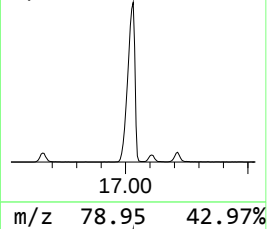
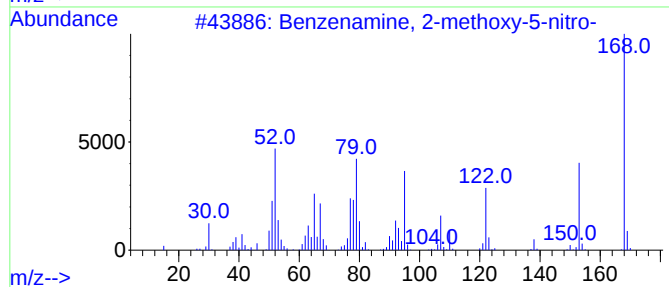
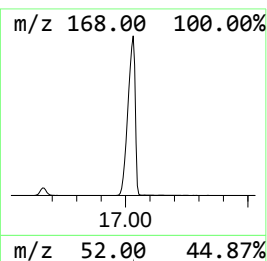
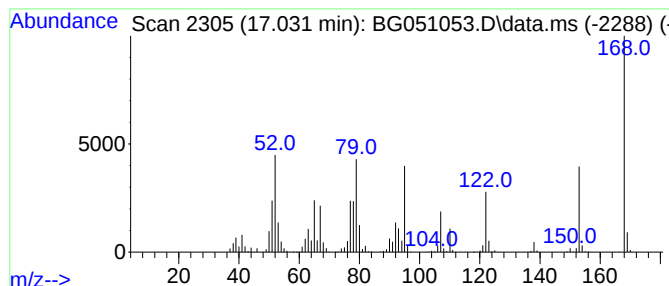
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.031	195.45 ng	6302370	Phenanthrene-d10	17.601

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	94
3		Benzenamine, 4-methoxy-2-nitro-	168	C7H8N2O3	000096-96-8	83
4		p-Anisidine, 3-nitro-,	168	C7H8N2O3	000577-72-0	72
5		Benzenamine, 3-methoxy-5-nitro-	168	C7H8N2O3	000586-10-7	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
Operator : CG/JU
Sample : M4573-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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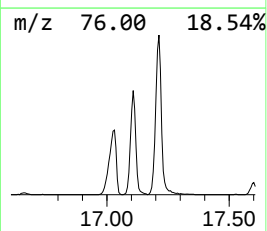
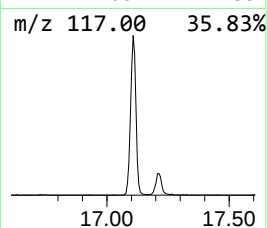
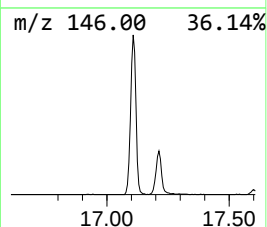
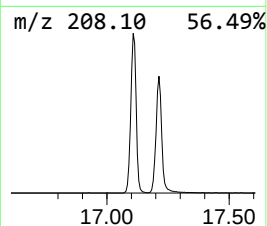
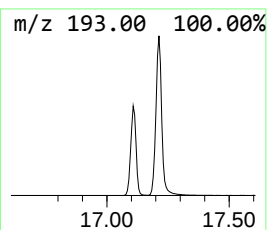
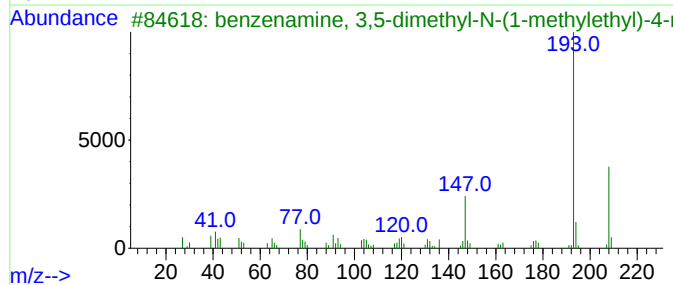
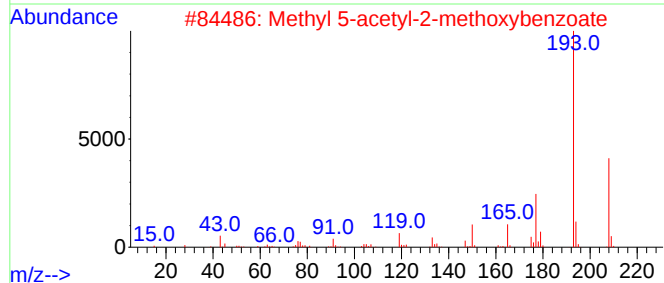
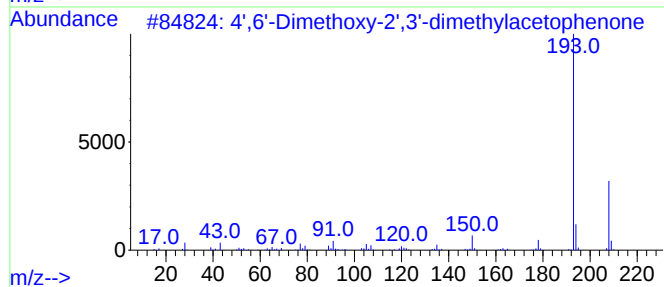
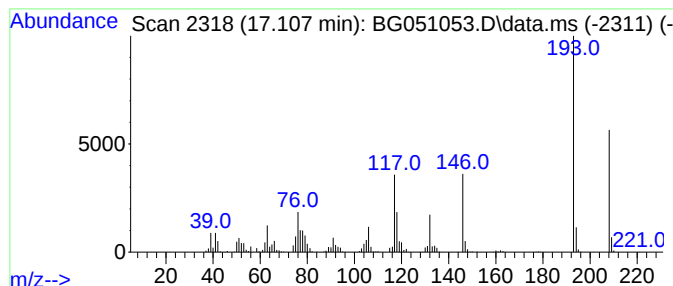
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 4',6'-Dimethoxy-2',3'-dimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.107	51.46 ng	1659460	Phenanthrene-d10	17.601

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4',6'-Dimethoxy-2',3'-dimethylac...	208	C12H16O3	1010244-80-3	53
2			Methyl 5-acetyl-2-methoxybenzoate	208	C11H12O4	039971-36-3	49
3			benzenamine, 3,5-dimethyl-N-(1-m...	208	C11H16N2O2	1000400-57-7	47
4			1H-Pyrazole, 1-methyl-4-(4,4,5,5...	208	C10H17BN2O2	1000319-69-0	47
5			2-Acetylthiophene, 5-(2-thienyl)-	208	C10H8OS2	003515-18-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
Operator : CG/JU
Sample : M4573-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

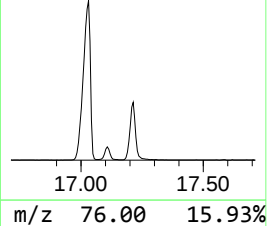
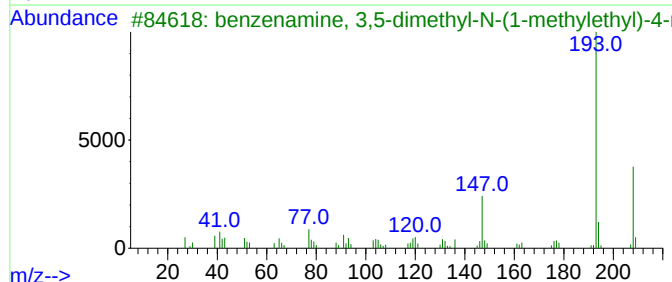
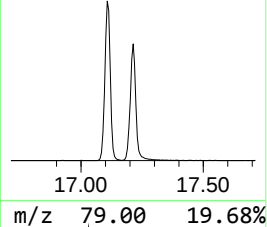
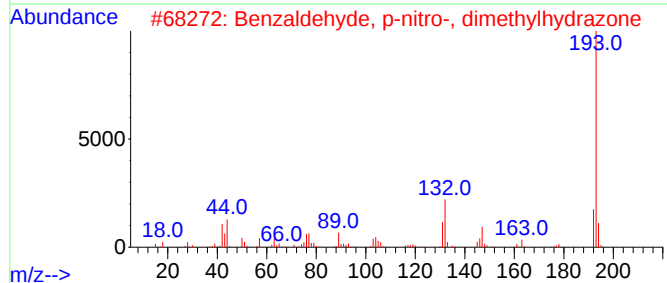
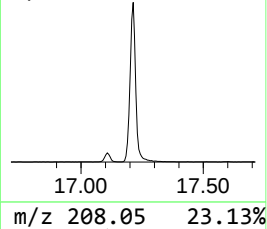
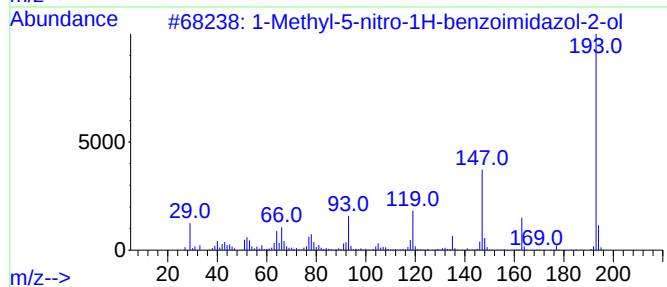
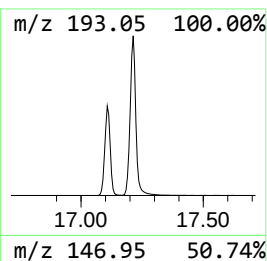
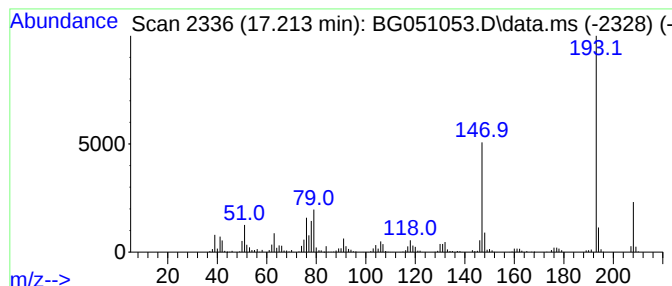
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1-Methyl-5-nitro-1H-benzoim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.213	84.57 ng	2727030	Phenanthrene-d10		17.601	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Methyl-5-nitro-1H-benzoimidazo...		193	C8H7N3O3	066108-85-8	58
2	Benzaldehyde, p-nitro-, dimethyl...		193	C9H11N3O2	010424-92-7	38
3	benzenamine, 3,5-dimethyl-N-(1-m...		208	C11H16N2O2	1000400-57-7	38
4	1H-benzimidazole-2-methanol, 6-n...		193	C8H7N3O3	1000400-27-2	32
5	Pyrazole, 5-methyl-3-(5-nitro-2-...		193	C8H7N3O3	016239-90-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
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Sample : M4573-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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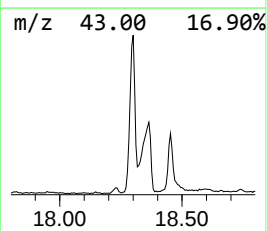
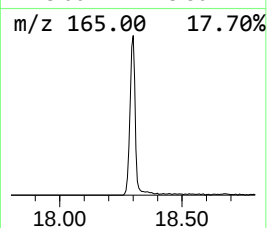
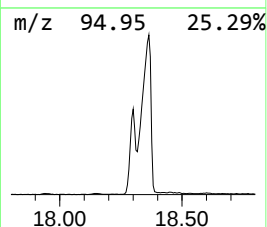
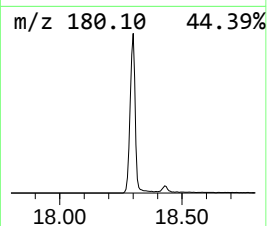
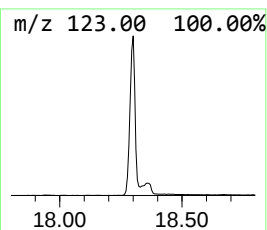
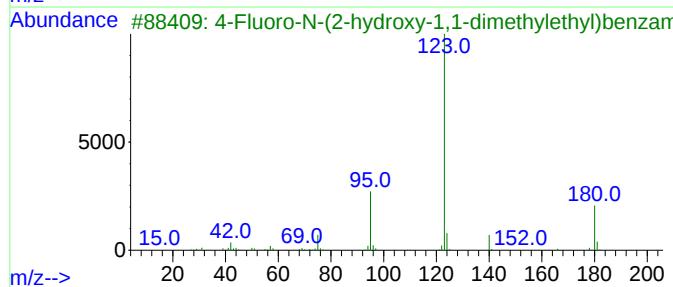
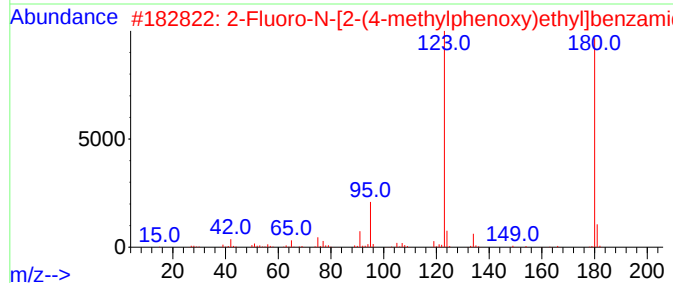
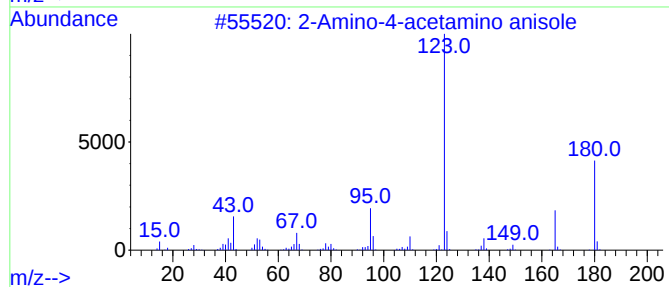
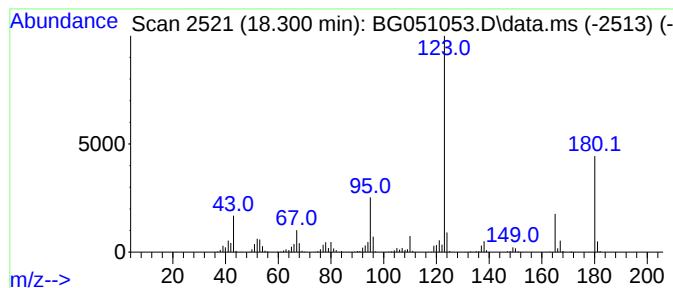
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 2-Amino-4-acetamino anisole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.300	47.23 ng	1522830	Phenanthrene-d10	17.601

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Amino-4-acetamino anisole	180	C9H12N2O2	006375-47-9	93
2			2-Fluoro-N-[2-(4-methylphenoxy)e...	287	C17H18FNO2	1178434-93-9	72
3			4-Fluoro-N-(2-hydroxy-1,1-dimeth...	211	C11H14FNO2	343316-37-0	64
4			4-Fluorobenzoic acid, allyl ester	180	C10H9FO2	329361-68-4	47
5			Benzhydrazide, 4-fluoro-N2-chlor...	230	C9H8ClFN2O2	1000266-55-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
Operator : CG/JU
Sample : M4573-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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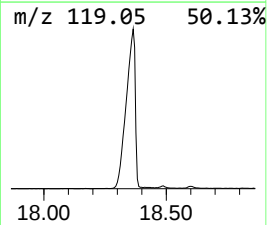
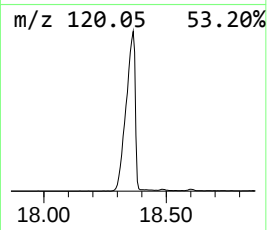
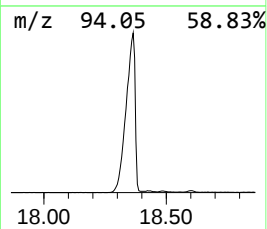
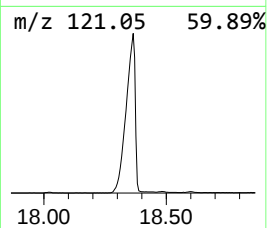
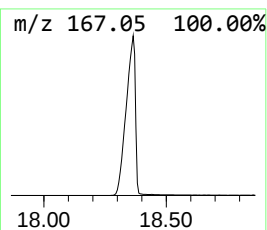
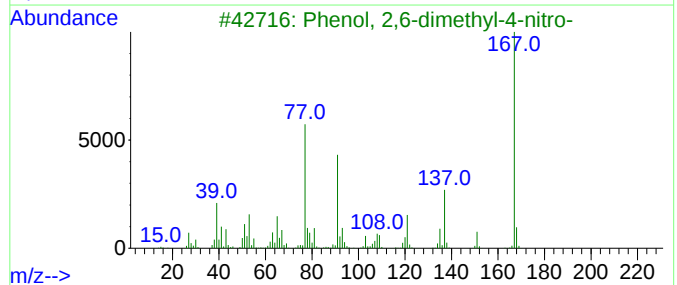
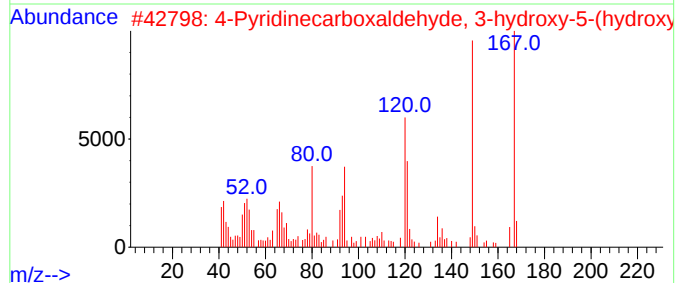
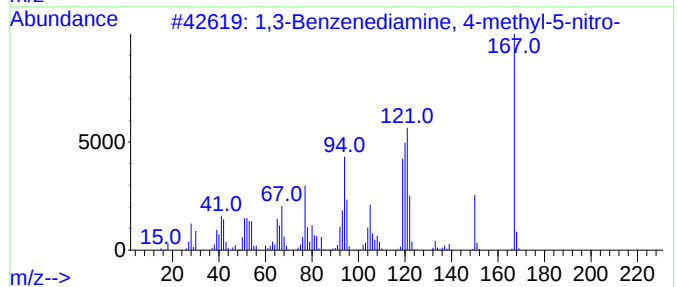
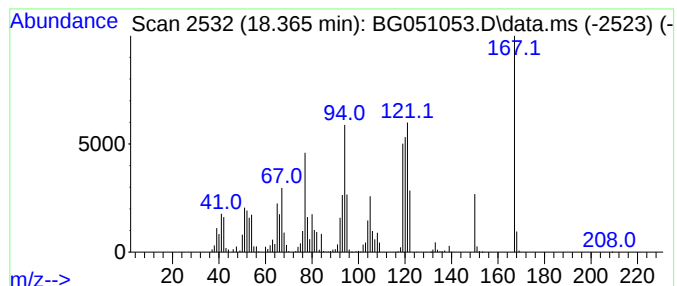
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.365	286.31 ng	9232290	Phenanthrene-d10	17.601

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenediamine, 4-methyl-5-n...	167	C7H9N3O2	006629-29-4	98
2			4-Pyridinecarboxaldehyde, 3-hydr...	167	C8H9NO3	000066-72-8	60
3			Phenol, 2,6-dimethyl-4-nitro-	167	C8H9NO3	002423-71-4	25
4			3,5-Pyridinedicarboxylic acid	167	C7H5NO4	000499-81-0	25
5			1H-Pyrrole-2-carboxylic acid, 3-...	167	C9H13NO2	069687-81-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
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Sample : M4573-01
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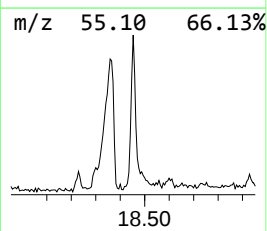
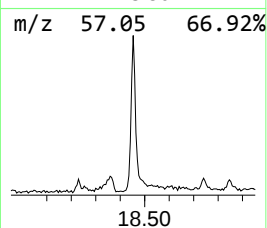
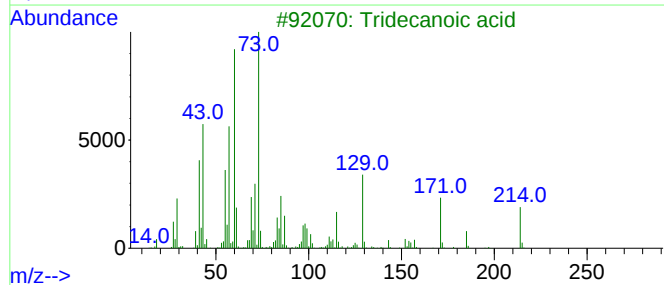
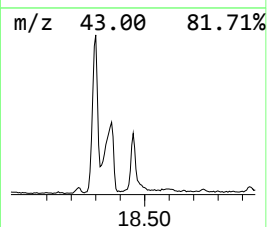
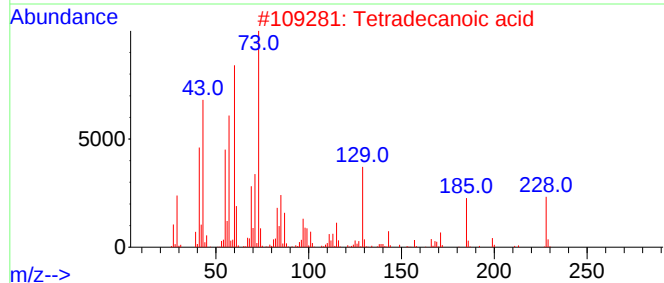
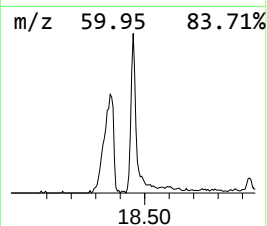
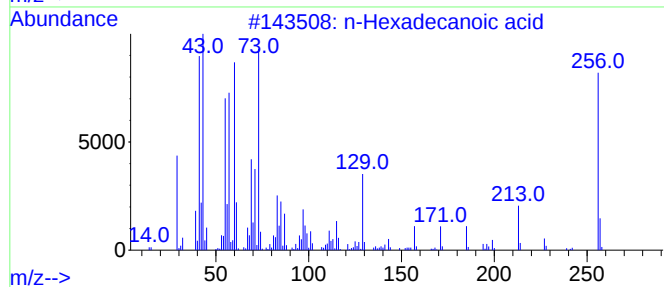
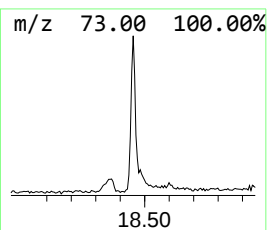
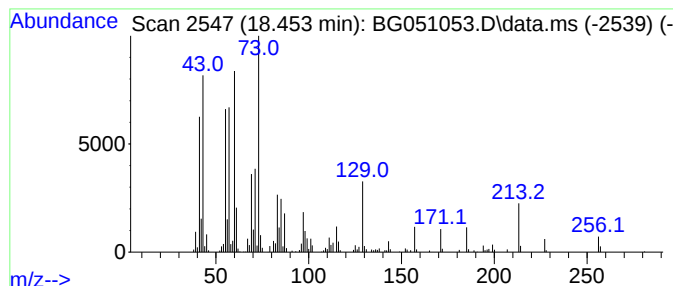
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 n-Hexadecanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.453	12.53 ng	404019	Phenanthrene-d10		17.601	
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	94
3	Tridecanoic acid		214	C13H26O2	000638-53-9	74
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	62
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
Operator : CG/JU
Sample : M4573-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

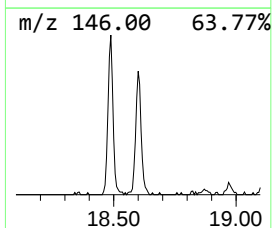
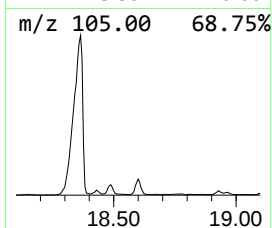
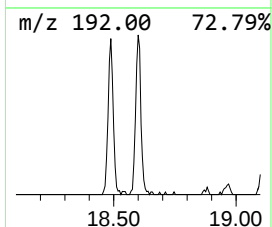
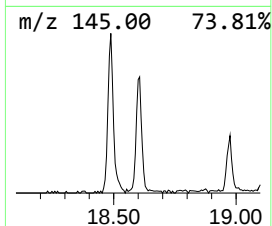
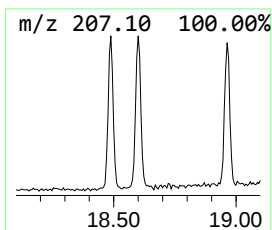
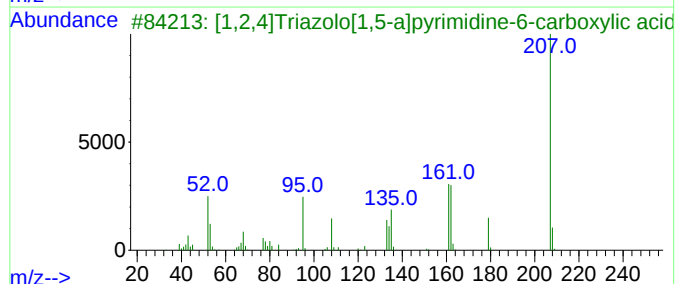
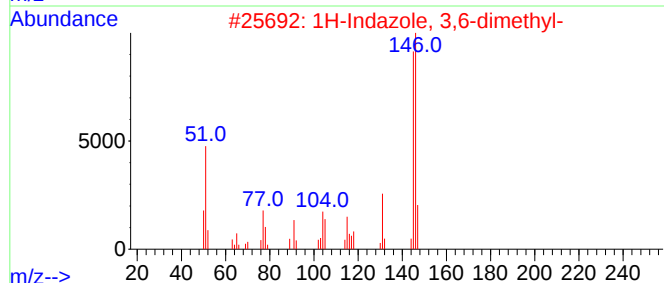
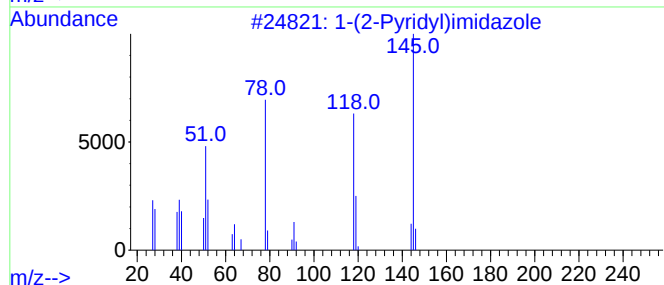
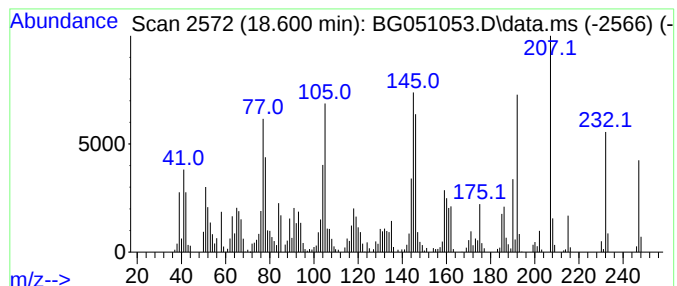
Instrument :
BNA_G
ClientSampleId :
MBR1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown18.599 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD			R.T.
18.599	13.75 ng	443357	Phenanthrene-d10			17.601
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-(2-Pyridyl)imidazole	145	C8H7N3	025700-14-5	38
2		1H-Indazole, 3,6-dimethyl-	146	C9H10N2	007746-28-3	38
3		[1,2,4]Triazolo[1,5-a]pyrimidine...	207	C8H9N5O2	092673-40-0	38
4		2,3-Dimethyl-1H-pyrrolo[2,3-b]py...	146	C9H10N2	010299-69-1	30
5		Benzene, 1-azido-3-methyl-	133	C7H7N3	004113-72-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051053.D
Acq On : 15 Nov 2021 22:49
Operator : CG/JU
Sample : M4573-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MBR1

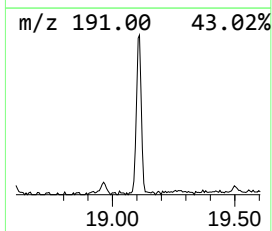
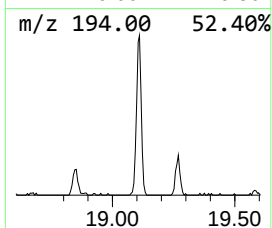
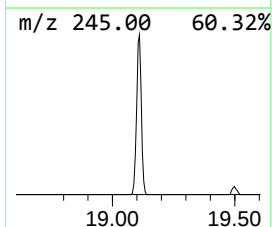
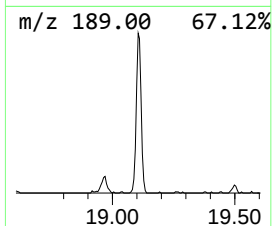
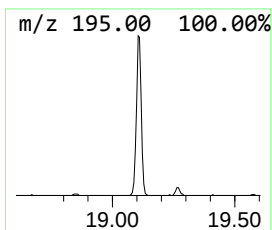
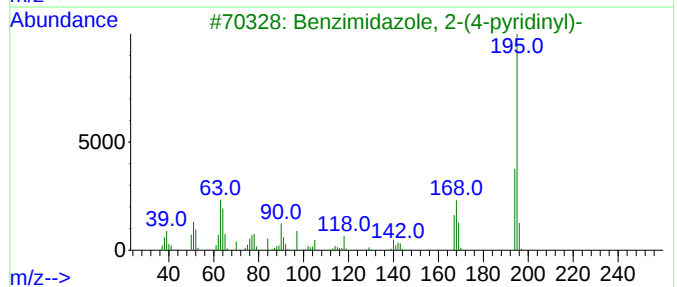
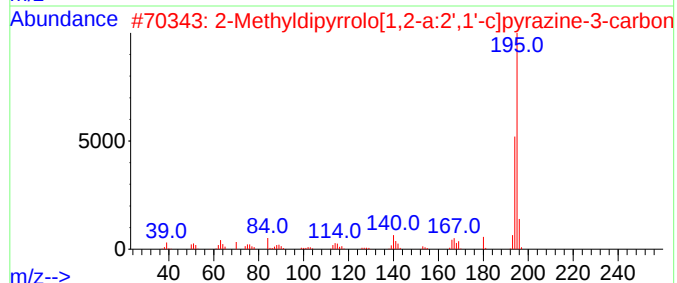
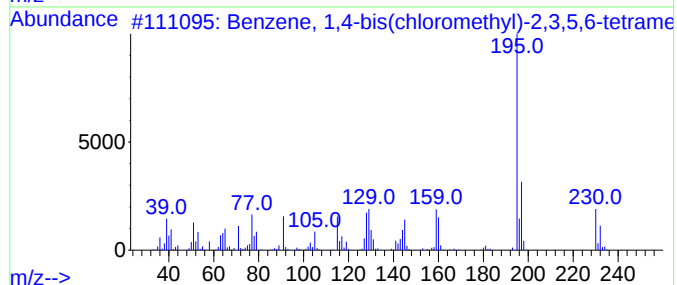
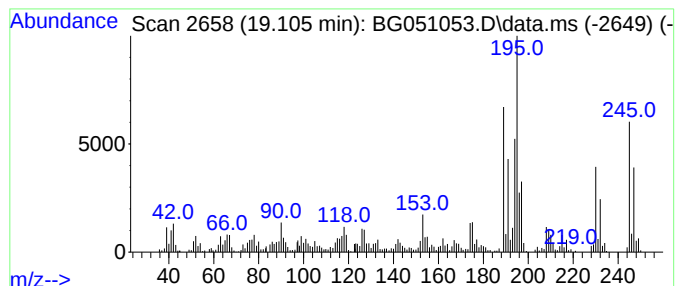
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown19.105 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.105	17.84 ng	575218	Phenanthrene-d10	17.601

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-bis(chloromethyl)-2...	230	C12H16Cl2	003022-16-0	42
2			2-Methyldipyrrolo[1,2-a:2',1'-c]...	195	C12H9N3	1010305-64-5	30
3			Benzimidazole, 2-(4-pyridinyl)-	195	C12H9N3	002208-59-5	25
4			4-Chloro-7-phenyl-1H-imidazo[4,5...	230	C11H7ClN4	1000286-12-1	25
5			Carbazole, 1,5-dimethyl-	195	C14H13N	051640-60-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
 Data File : BG051053.D
 Acq On : 15 Nov 2021 22:49
 Operator : CG/JU
 Sample : M4573-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MBR1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.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
Propanoic acid,...	4.034	36.0	ng	458440	1	8.223	254376	20.0
Butanoic acid	4.322	16.7	ng	212694	1	8.223	254376	20.0
Butanoic acid, ...	5.245	142.0	ng	1805910	1	8.223	254376	20.0
Pentanoic acid,...	5.409	77.8	ng	990176	1	8.223	254376	20.0
3-Methyl-hexano...	8.282	17.1	ng	217582	1	8.223	254376	20.0
Hexanoic acid, ...	8.523	77.5	ng	986131	1	8.223	254376	20.0
Heptanoic acid	8.858	23.1	ng	294218	1	8.223	254376	20.0
Phenylethyl Alc...	9.780	18.5	ng	332433	2	11.050	358931	20.0
Ethanol, 2-(2-b...	10.797	17.6	ng	316338	2	11.050	358931	20.0
Benzeneacetic acid	11.631	42.6	ng	764550	2	11.050	358931	20.0
unknown12.659	12.659	24.6	ng	441115	2	11.050	358931	20.0
1,3-Benzenediam...	14.616	18.1	ng	497903	3	14.851	549875	20.0
Benzenamine, 2-...	17.031	195.4	ng	6302370	4	17.601	644923	20.0
4',6'-Dimethoxy...	17.107	51.5	ng	1659460	4	17.601	644923	20.0
1-Methyl-5-nitr...	17.213	84.6	ng	2727030	4	17.601	644923	20.0
2-Amino-4-aceta...	18.300	47.2	ng	1522830	4	17.601	644923	20.0
1,3-Benzenediam...	18.365	286.3	ng	9232290	4	17.601	644923	20.0
n-Hexadecanoic ...	18.453	12.5	ng	404019	4	17.601	644923	20.0
unknown18.599	18.599	13.8	ng	443357	4	17.601	644923	20.0
unknown19.105	19.105	17.8	ng	575218	4	17.601	644923	20.0