

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
 Data File : BG057645.D
 Acq On : 6 Jun 2023 20:16
 Operator : CG/JU
 Sample : 02997-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DMA-1103

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-BG052723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057645.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.990	68	77	86	rBV2	28764	69877	4.83%	0.529%
2	4.360	131	140	143	rBV	30804	62673	4.33%	0.474%
3	4.407	143	148	157	rVB	63194	98219	6.78%	0.743%
4	5.241	271	290	301	rBV	78599	340099	23.48%	2.573%
5	5.394	301	316	327	rVB2	60098	190717	13.17%	1.443%
6	5.858	375	395	407	rBV2	143615	392371	27.09%	2.969%
7	6.116	434	439	446	rBV	24221	37084	2.56%	0.281%
8	6.281	462	467	476	rBV	49551	78185	5.40%	0.592%
9	6.774	535	551	559	rBV	54786	170310	11.76%	1.289%
10	7.461	645	668	670	rBV2	113949	493253	34.06%	3.732%
11	7.491	670	673	685	rVB3	93259	203111	14.02%	1.537%
12	8.301	802	811	813	rBV2	23049	38830	2.68%	0.294%
13	8.337	813	817	822	rVV	69929	118562	8.19%	0.897%
14	8.384	822	825	829	rVV	11108	16633	1.15%	0.126%
15	8.971	916	925	935	rBV2	53206	129870	8.97%	0.983%
16	9.112	941	949	962	rBV	490303	879090	60.70%	6.651%
17	9.523	1011	1019	1027	rBV	206278	375112	25.90%	2.838%
18	9.658	1036	1042	1055	rBV	42689	93718	6.47%	0.709%
19	10.187	1127	1132	1138	rBV2	10594	21026	1.45%	0.159%
20	10.557	1177	1195	1211	rBV3	186926	661762	45.69%	5.007%
21	10.939	1253	1260	1271	rBV7	15301	39278	2.71%	0.297%
22	11.174	1293	1300	1310	rBV	107297	197076	13.61%	1.491%
23	11.667	1378	1384	1390	rBV	51424	90931	6.28%	0.688%
24	11.767	1390	1401	1408	rVV2	146718	455198	31.43%	3.444%
25	11.973	1430	1436	1447	rBV3	32779	69528	4.80%	0.526%
26	12.155	1463	1467	1477	rVB8	6464	14701	1.02%	0.111%
27	12.643	1543	1550	1557	rBV	141460	246341	17.01%	1.864%
28	12.966	1598	1605	1619	rBV	106269	226209	15.62%	1.712%
29	13.248	1647	1653	1663	rBV	96929	168707	11.65%	1.276%
30	13.377	1671	1675	1691	rVB4	26624	70853	4.89%	0.536%
31	13.577	1700	1709	1716	rVB	689112	1036840	71.59%	7.845%
32	13.817	1741	1750	1754	rVB	20957	37715	2.60%	0.285%
33	13.958	1767	1774	1783	rBV9	7275	22636	1.56%	0.171%
34	14.352	1833	1841	1845	rBV6	9841	22530	1.56%	0.170%
35	14.605	1877	1884	1891	rVB2	14798	27327	1.89%	0.207%
36	14.687	1892	1898	1903	rBV3	8196	15259	1.05%	0.115%

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.769	1905	1912	1919	rBV	59490	102646	7.09%	0.777%
38	14.957	1937	1944	1950	rVB	197969	309393	21.36%	2.341%
39	15.233	1986	1991	1995	rBV	148020	218283	15.07%	1.652%
40	15.268	1995	1997	2004	rVV	62768	92569	6.39%	0.700%
41	15.333	2004	2008	2021	rVB	50022	90061	6.22%	0.681%
42	15.680	2060	2067	2073	rBV	96387	167029	11.53%	1.264%
43	15.733	2073	2076	2080	rVB2	11755	16402	1.13%	0.124%
44	15.909	2102	2106	2115	rBV8	7762	16793	1.16%	0.127%
45	16.226	2156	2160	2164	rVV2	16217	22570	1.56%	0.171%
46	16.291	2164	2171	2179	rVV	58945	100177	6.92%	0.758%
47	16.437	2190	2196	2208	rBV	526384	836682	57.77%	6.330%
48	16.567	2210	2218	2223	rVV	51426	78668	5.43%	0.595%
49	16.637	2226	2230	2236	rVB2	16287	28002	1.93%	0.212%
50	16.755	2243	2250	2254	rBV7	11784	23725	1.64%	0.180%
51	16.843	2261	2265	2274	rVB7	10053	17063	1.18%	0.129%
52	17.019	2290	2295	2297	rBV3	13273	18964	1.31%	0.143%
53	17.048	2297	2300	2304	rVV	64469	92232	6.37%	0.698%
54	17.095	2304	2308	2321	rVB3	40899	75400	5.21%	0.570%
55	17.330	2343	2348	2355	rBV7	11326	27116	1.87%	0.205%
56	17.542	2381	2384	2388	rVV3	10907	15151	1.05%	0.115%
57	17.606	2391	2395	2401	rVV7	12604	22270	1.54%	0.168%
58	17.695	2404	2410	2418	rVB	262943	398455	27.51%	3.015%
59	17.818	2425	2431	2437	rBV8	14697	28685	1.98%	0.217%
60	17.900	2441	2445	2456	rVV6	30832	65630	4.53%	0.497%
61	17.994	2456	2461	2471	rVV2	45433	105893	7.31%	0.801%
62	18.112	2476	2481	2489	rVB	21145	37716	2.60%	0.285%
63	18.435	2531	2536	2548	rBV5	17971	41970	2.90%	0.318%
64	18.535	2548	2553	2563	rBV	208384	316718	21.87%	2.396%
65	19.099	2645	2649	2652	rBV3	11405	15850	1.09%	0.120%
66	19.292	2677	2682	2686	rBV2	42653	65673	4.53%	0.497%
67	19.786	2762	2766	2774	rBV4	33360	54141	3.74%	0.410%
68	20.262	2841	2847	2858	rBV	1096442	1448223	100.00%	10.957%
69	20.432	2874	2876	2882	rVB7	15640	18060	1.25%	0.137%
70	21.008	2970	2974	2979	rBV	53149	67473	4.66%	0.511%
71	21.572	3064	3070	3080	rBV5	39589	104013	7.18%	0.787%
72	22.000	3137	3143	3151	rVB	228132	403725	27.88%	3.055%
73	23.175	3337	3343	3344	rBV6	15265	27548	1.90%	0.208%
74	23.716	3431	3435	3441	rVB2	18468	32230	2.23%	0.244%
75	25.490	3728	3737	3750	rVB2	131516	402144	27.77%	3.043%

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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-BG052723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

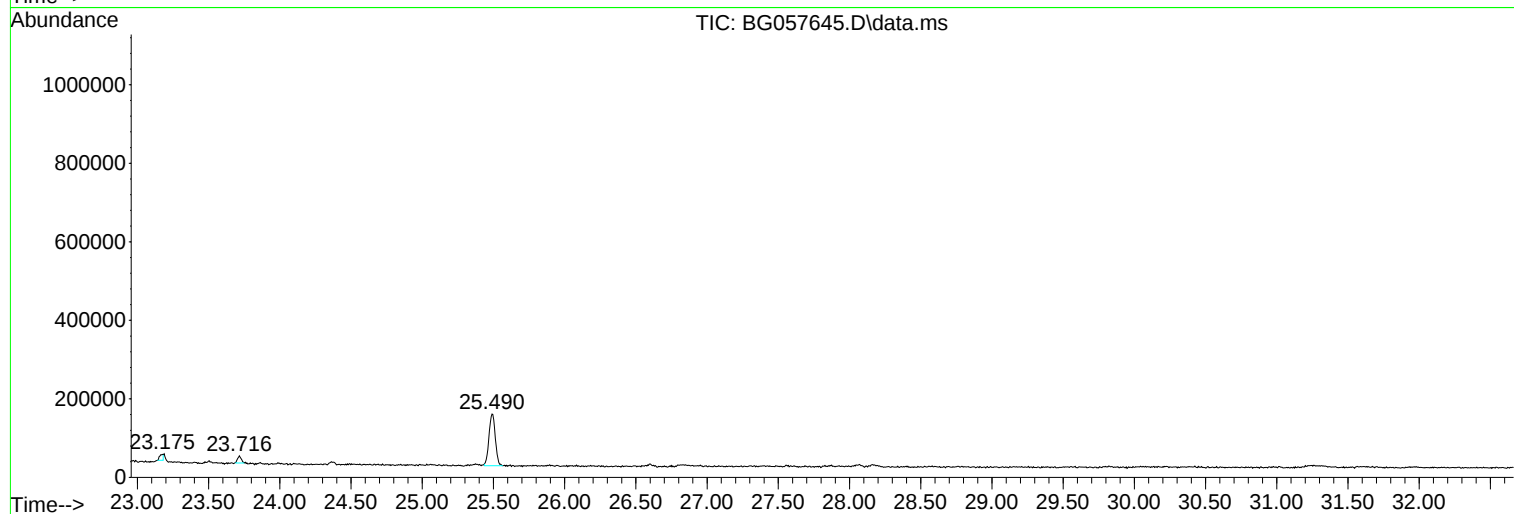
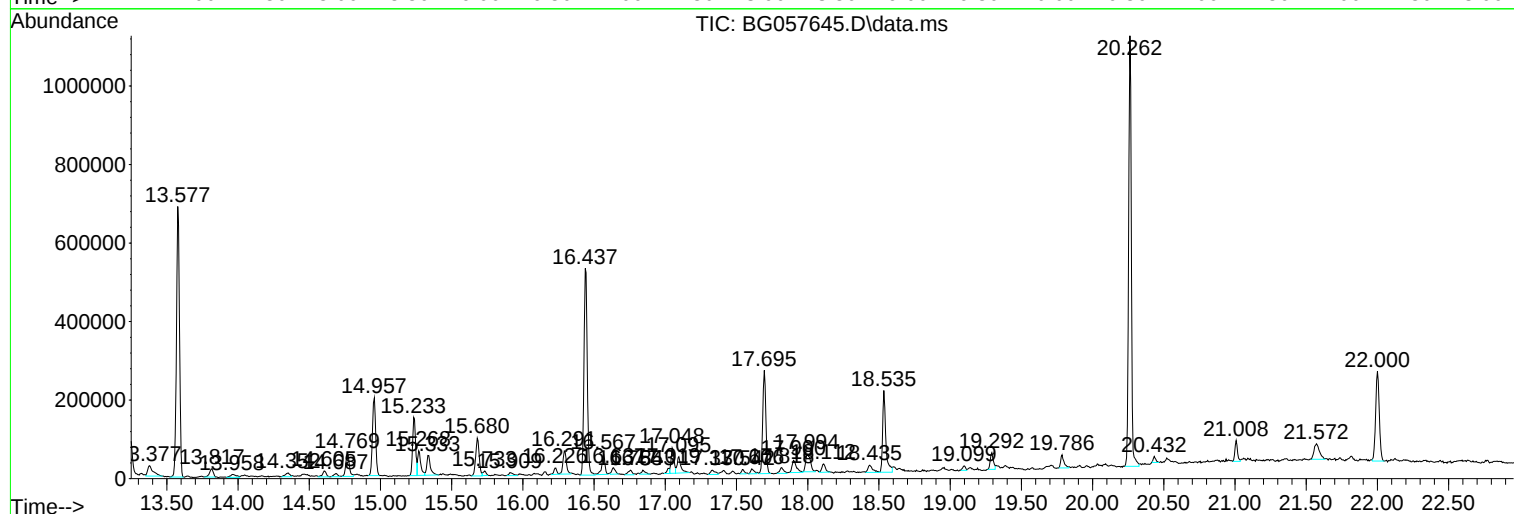
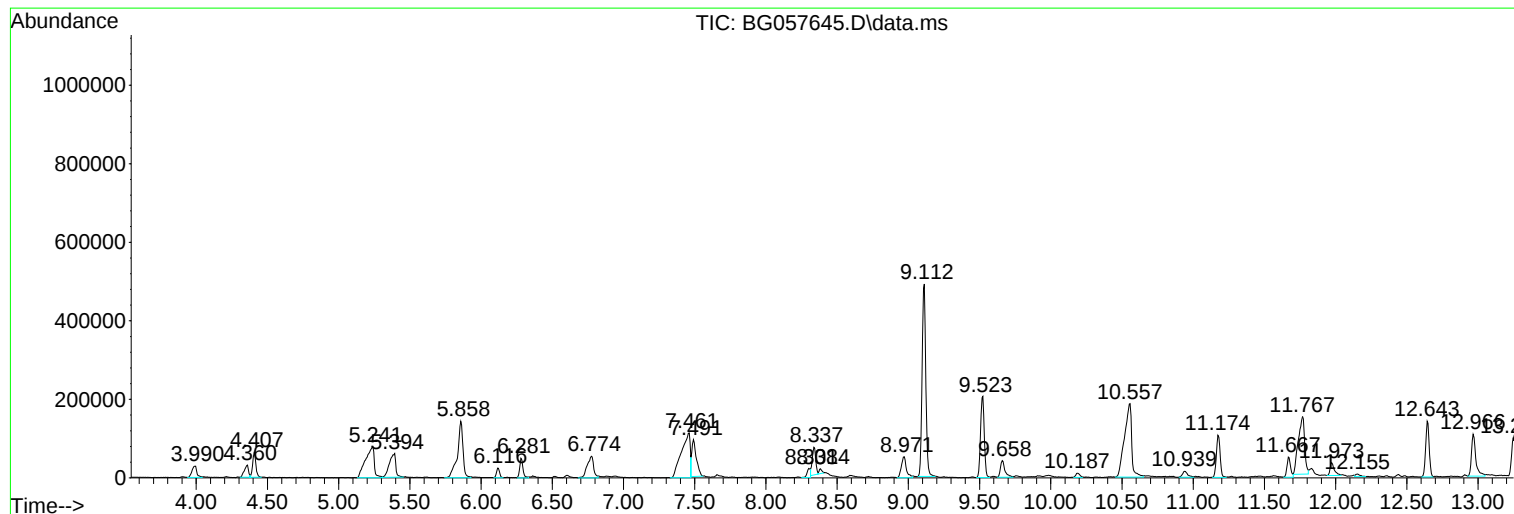
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Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
Operator : CG/JU
Sample : 02997-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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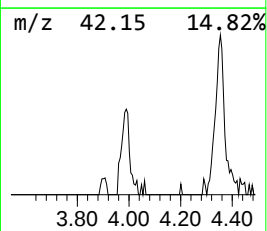
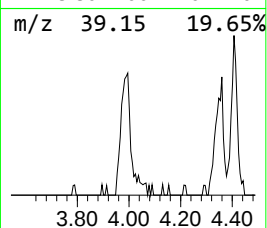
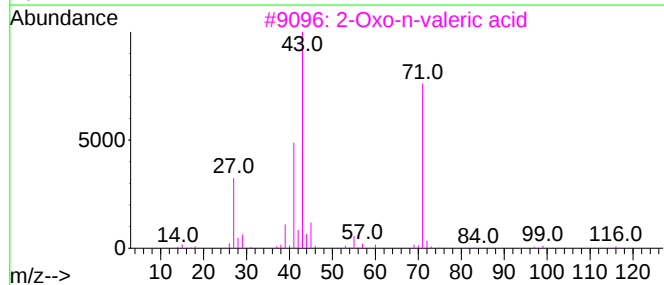
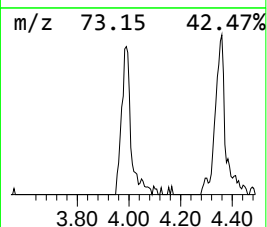
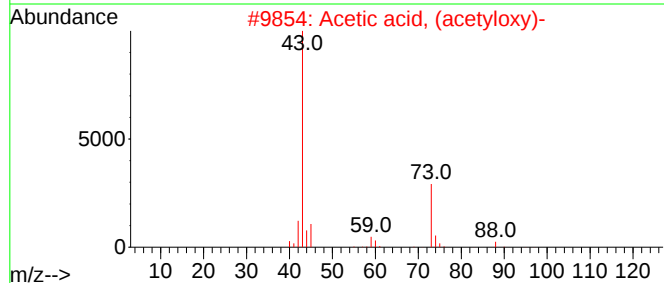
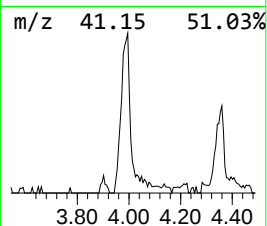
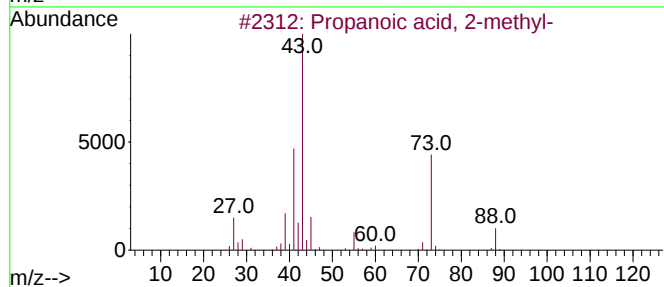
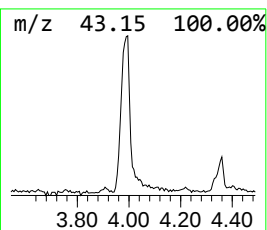
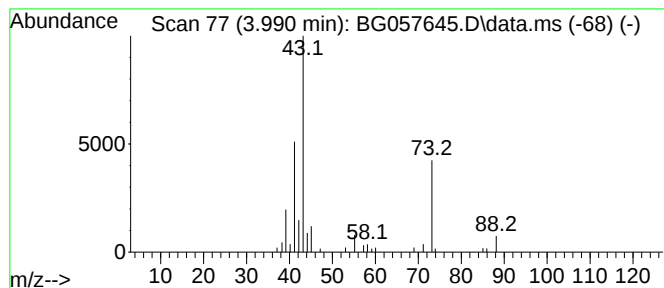
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.990	11.79 ng	69877	1,4-Dichlorobenzene-d4	8.337

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	90
2			Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	38
3			2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	38
4			N-Acetythylenediamine	102	C4H10N2O	001001-53-2	36
5			N,N'-Diacythylenediamine	144	C6H12N2O2	000871-78-3	36



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ALS Vial : 11 Sample Multiplier: 1

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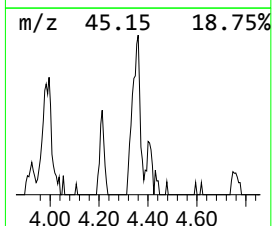
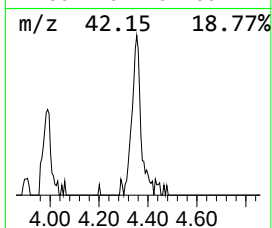
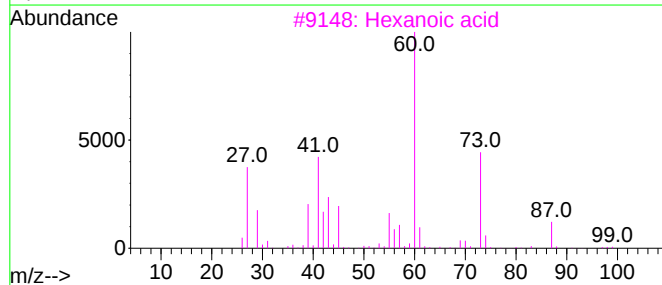
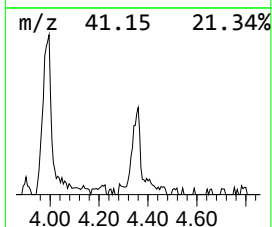
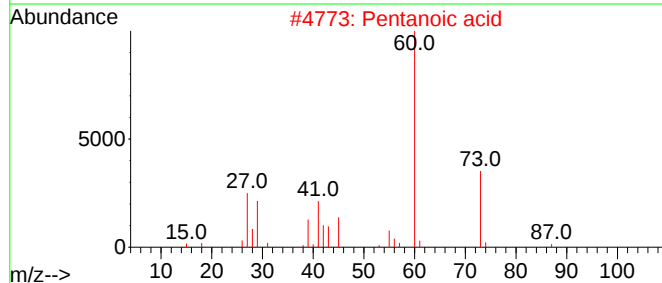
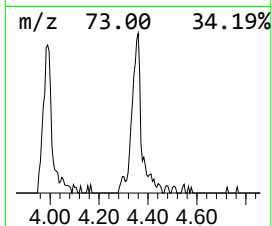
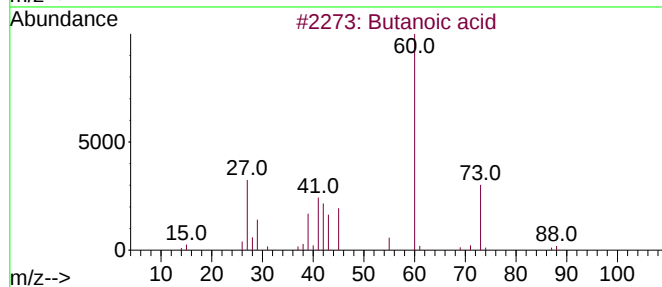
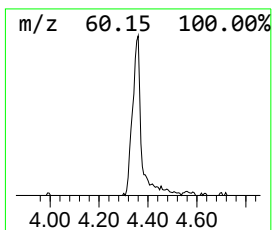
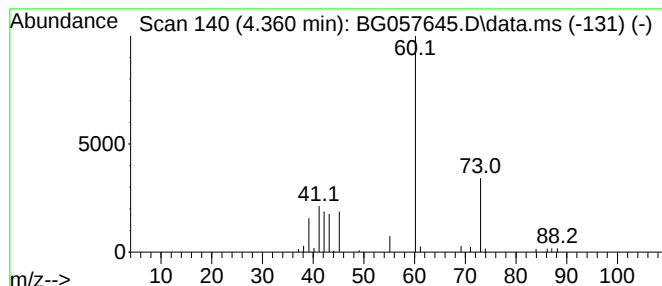
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.360	10.57 ng	62673	1,4-Dichlorobenzene-d4	8.337

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	64
3			Hexanoic acid	116	C6H12O2	000142-62-1	40
4			Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	38
5			4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9



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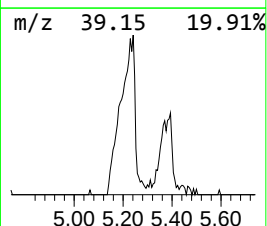
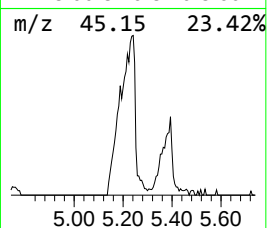
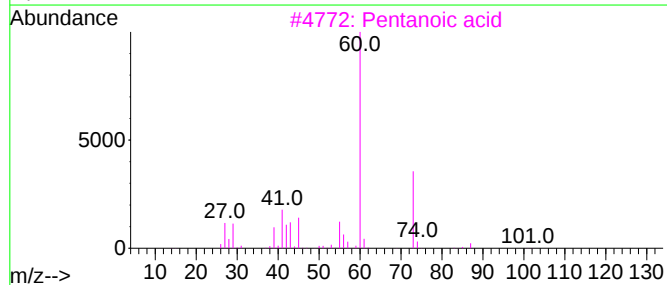
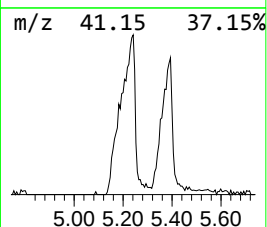
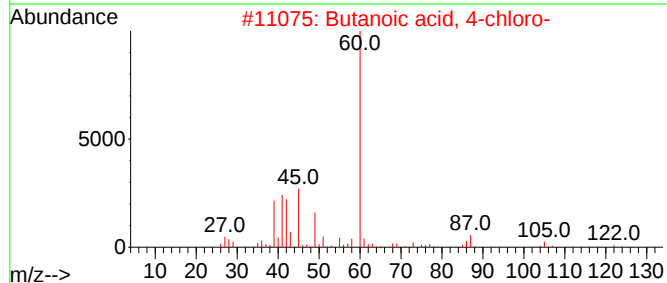
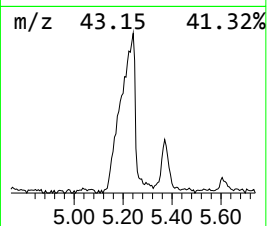
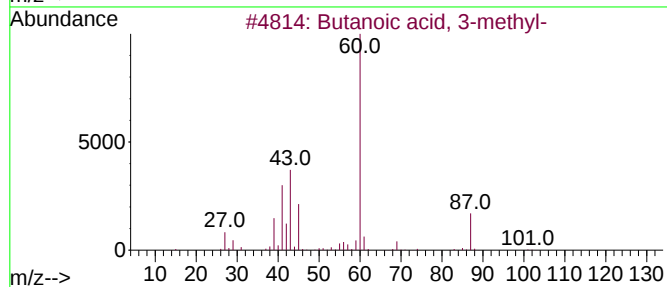
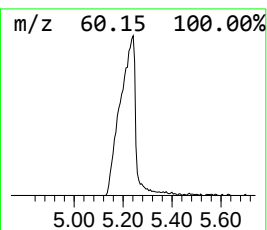
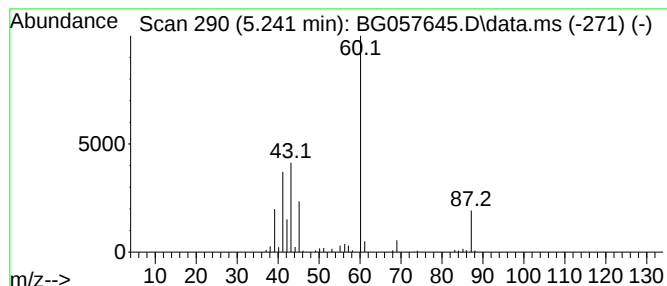
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Butanoic acid, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.241	57.37 ng	340099	1,4-Dichlorobenzene-d4	8.337

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	90
2			Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	38
3			Pentanoic acid	102	C5H10O2	000109-52-4	36
4			Formic acid hydrazide	60	CH4N2O	000624-84-0	28
5			Ethylamine	45	C2H7N	000075-04-7	7



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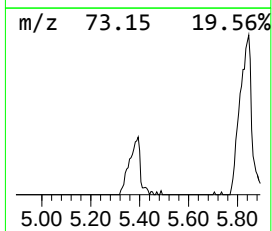
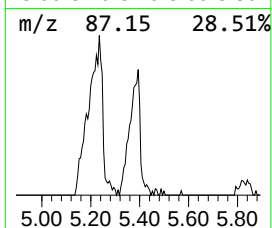
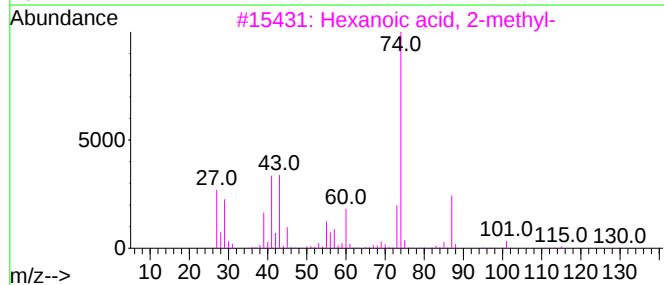
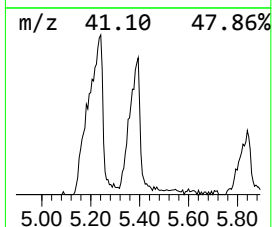
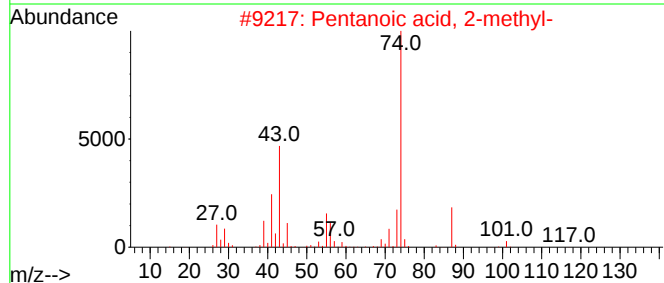
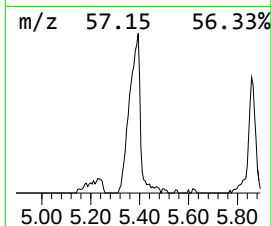
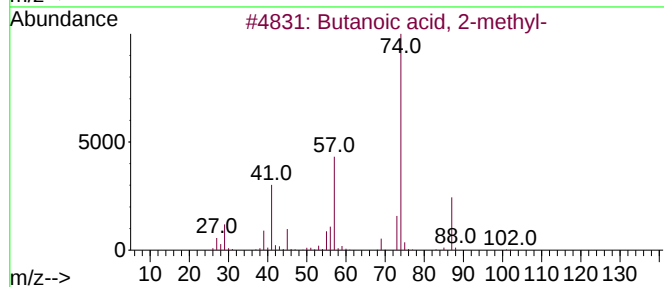
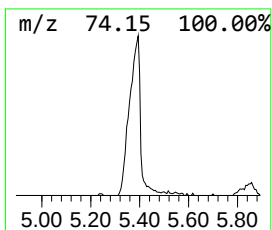
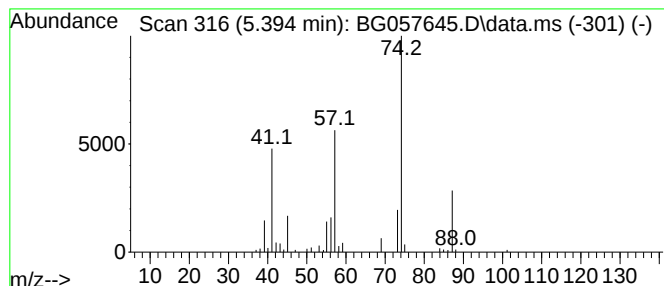
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.394	32.17 ng	190717	1,4-Dichlorobenzene-d4	8.337

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
2			Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	56
3			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	43
4			1,2-Butanediol, 3,3-dimethyl-	118	C6H14O2	059562-82-2	22
5			Morpholine	87	C4H9NO	000110-91-8	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
Operator : CG/JU
Sample : 02997-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DMA-1103

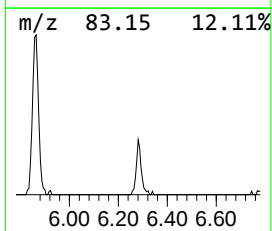
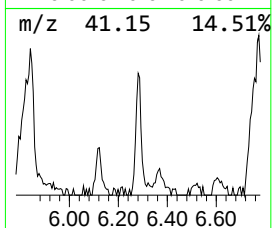
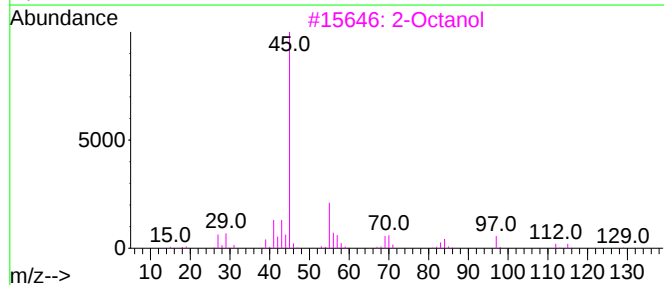
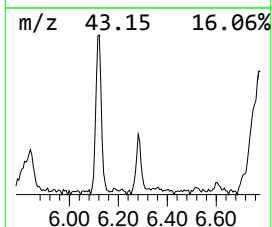
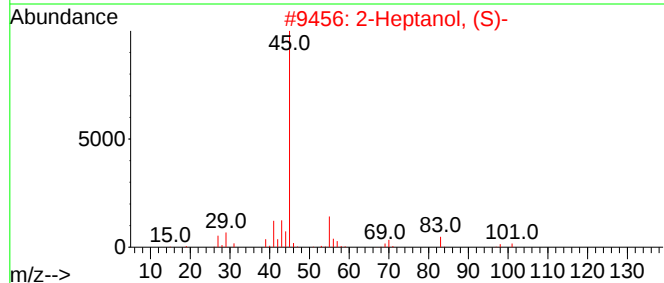
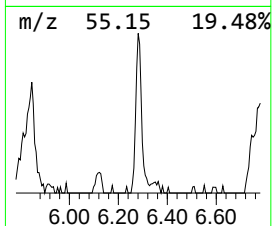
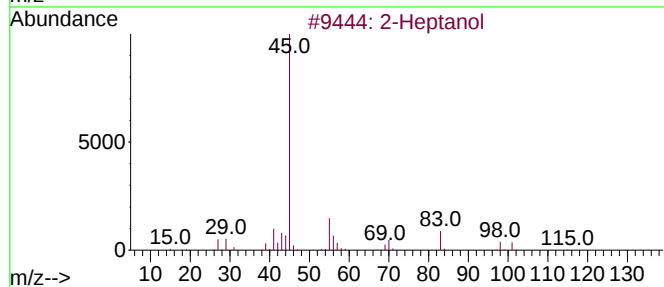
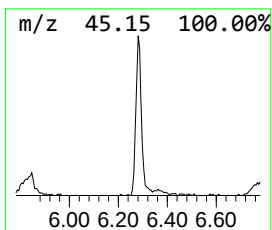
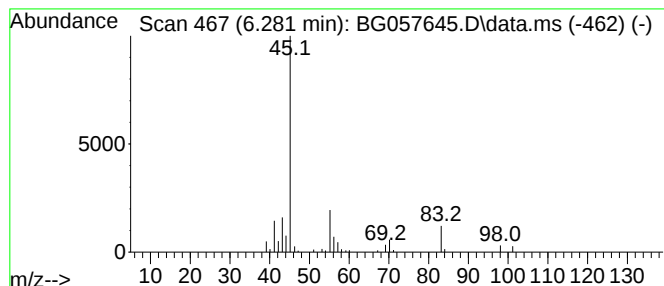
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Heptanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.281	13.19 ng	78185	1,4-Dichlorobenzene-d4	8.337

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanol	116	C7H16O	000543-49-7	83
2			2-Heptanol, (S)-	116	C7H16O	006033-23-4	78
3			2-Octanol	130	C8H18O	000123-96-6	72
4			2-Octanol, (R)-	130	C8H18O	005978-70-1	72
5			Butane, 1-methoxy-3-methyl-	102	C6H14O	000626-91-5	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
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Sample : 02997-01
Misc :
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ClientSampleId :
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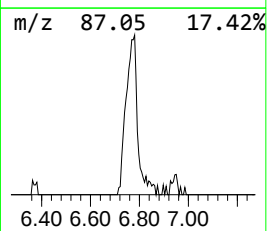
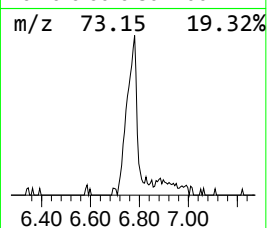
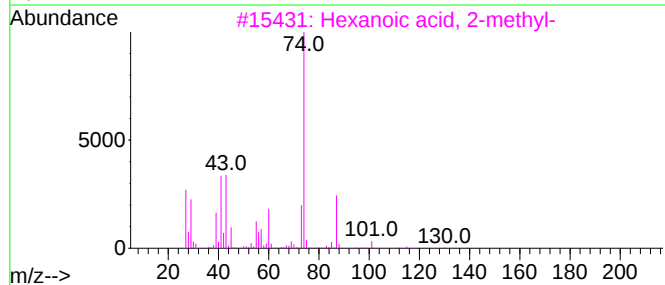
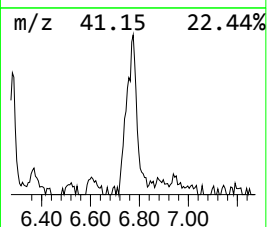
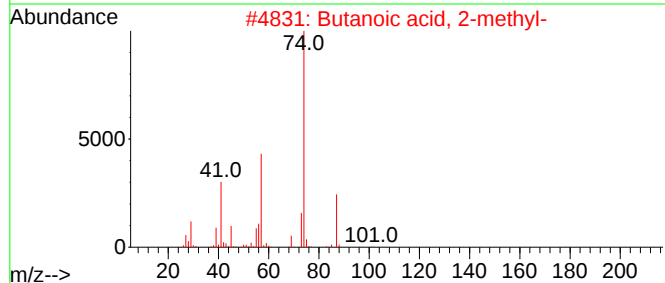
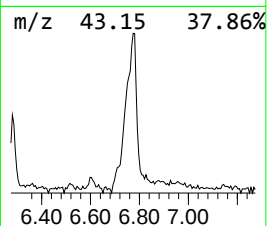
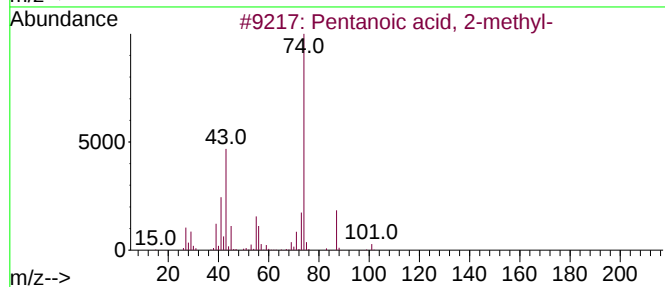
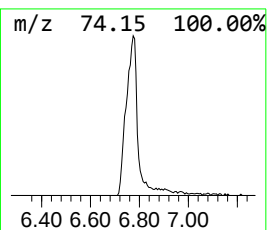
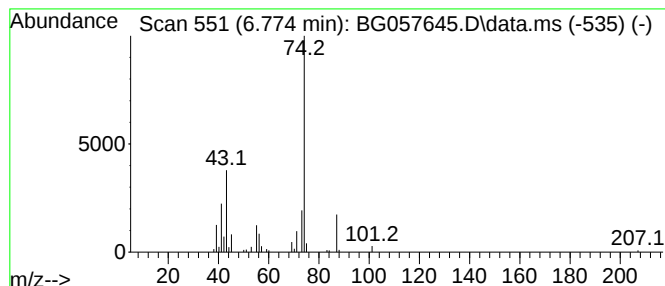
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentanoic acid, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.774	28.73 ng	170310	1,4-Dichlorobenzene-d4	8.337

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	83
2			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	72
3			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	56
4			3-(Dioxolan-2-yl)-1,1-dimethyl-2...	251	C14H21NO3	1000305-98-1	36
5			Undecanoic acid, 2-methyl-	200	C12H24O2	024323-25-9	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
Operator : CG/JU
Sample : 02997-01
Misc :
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Instrument :
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ClientSampleId :
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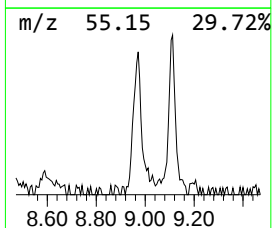
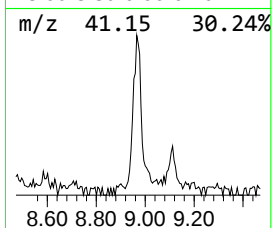
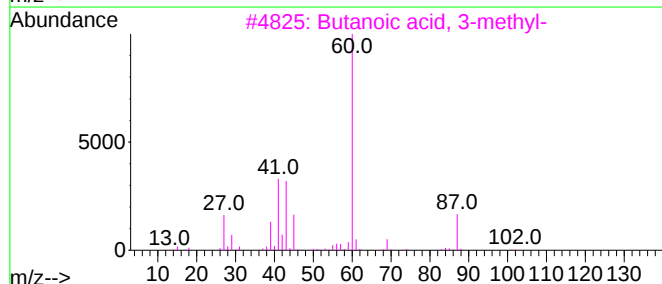
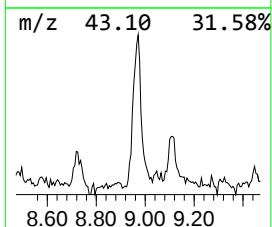
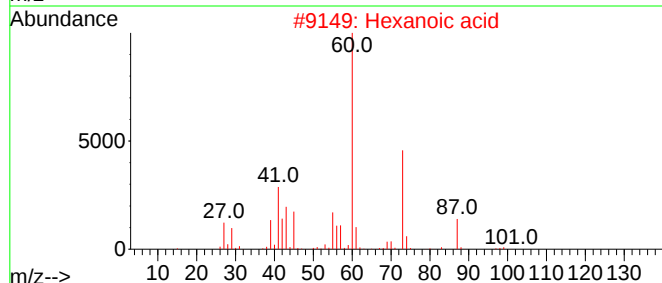
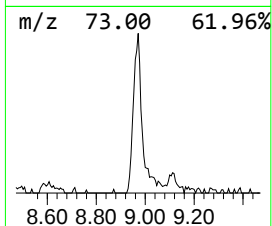
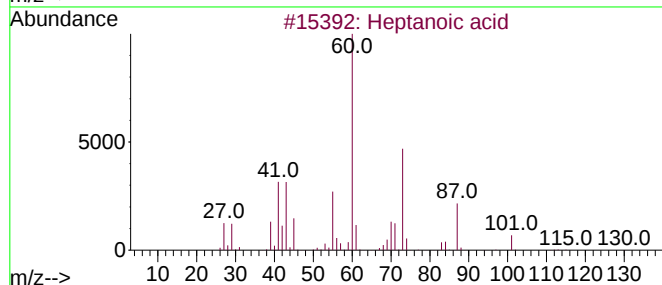
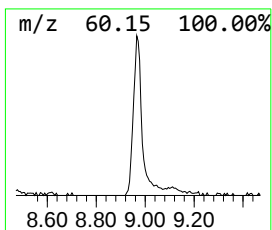
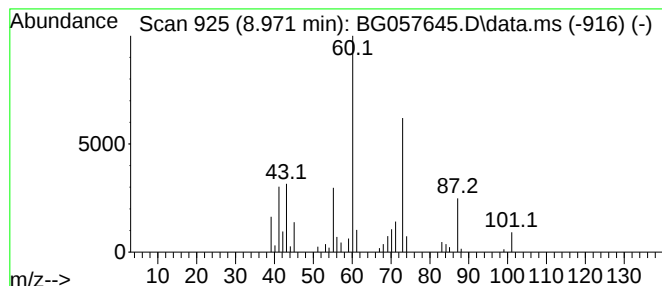
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.971	21.91 ng	129870	1,4-Dichlorobenzene-d4	8.337

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	59
4			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	45
5			3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
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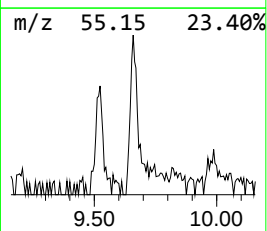
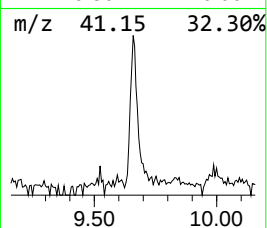
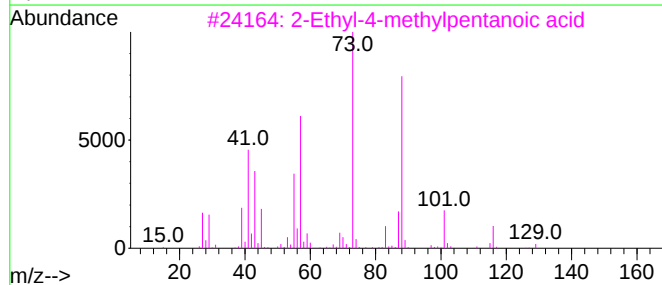
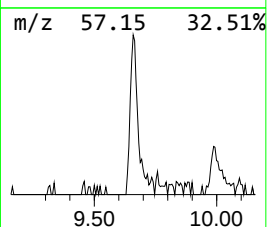
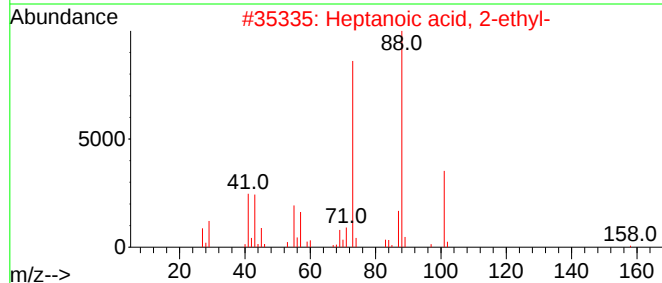
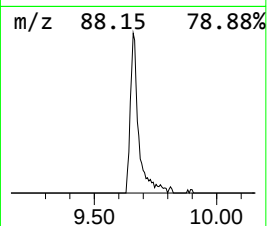
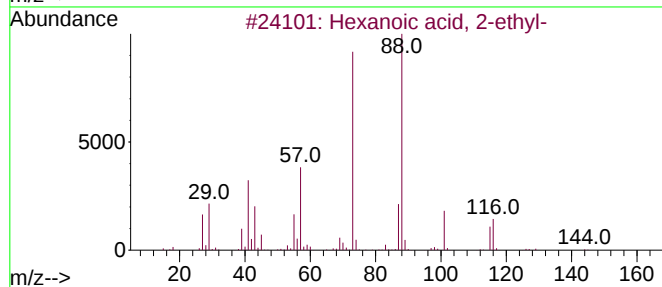
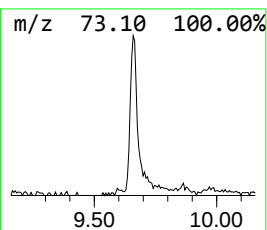
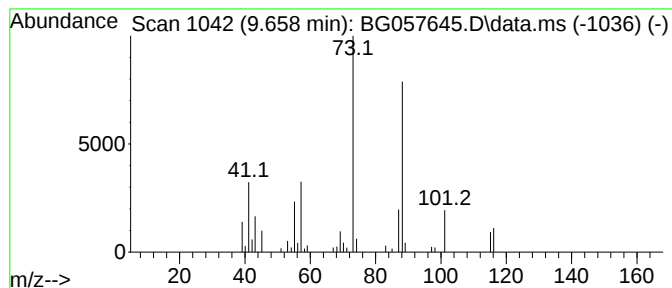
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexanoic acid, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.658	15.81 ng	93718	1,4-Dichlorobenzene-d4	8.337

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
3			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	42
4			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
5			1,4-Dioxane	88	C4H8O2	000123-91-1	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
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Sample : 02997-01
Misc :
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ClientSampleId :
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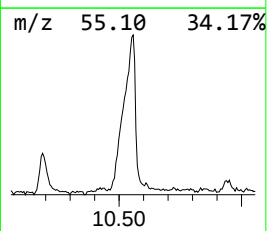
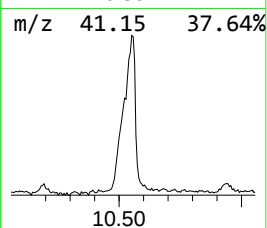
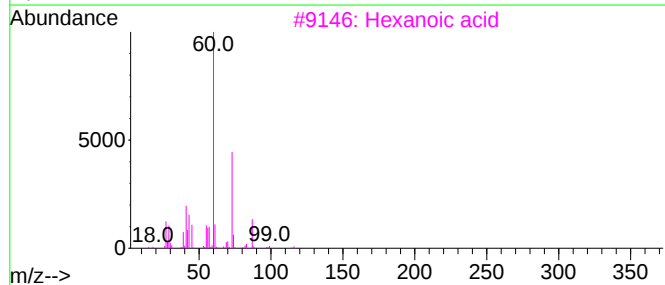
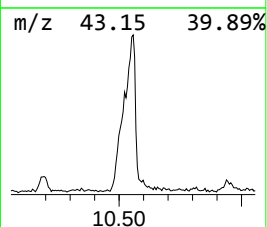
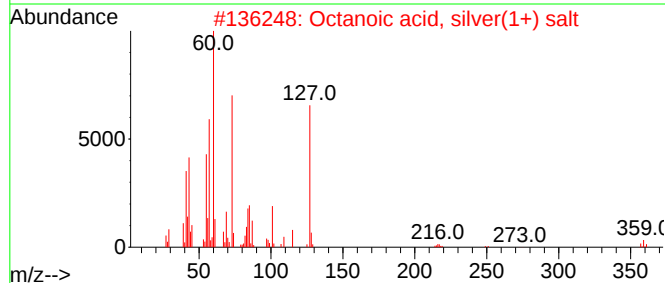
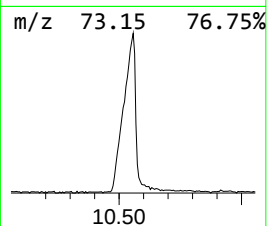
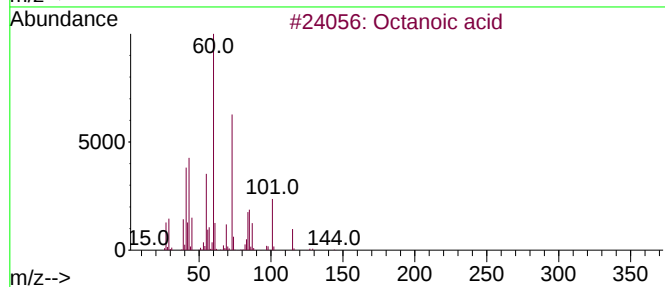
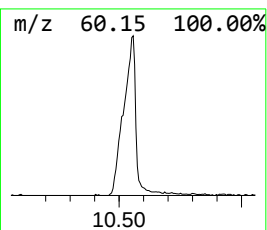
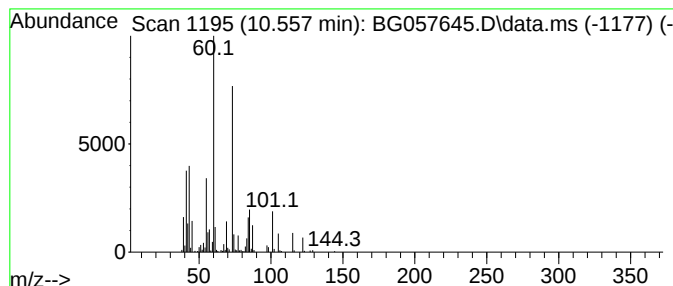
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.557	67.16 ng	661762	Naphthalene-d8	11.174

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octanoic acid	144	C8H16O2	000124-07-2	95
2		Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	86
3		Hexanoic acid	116	C6H12O2	000142-62-1	53
4		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	40
5		Heptanoic acid	130	C7H14O2	000111-14-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
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Sample : 02997-01
Misc :
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ClientSampleId :
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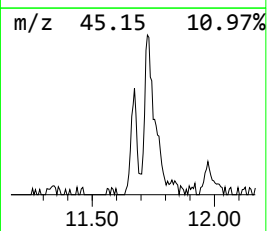
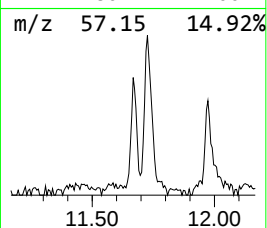
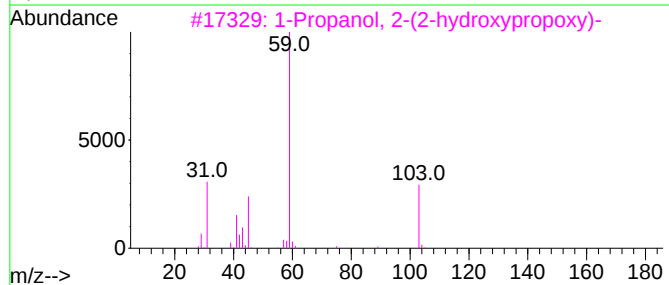
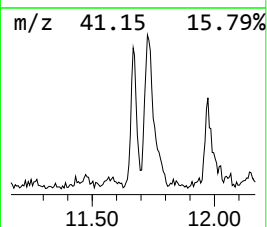
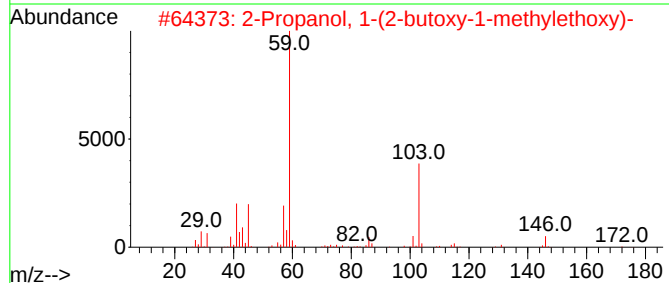
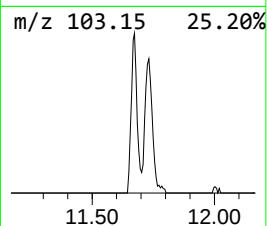
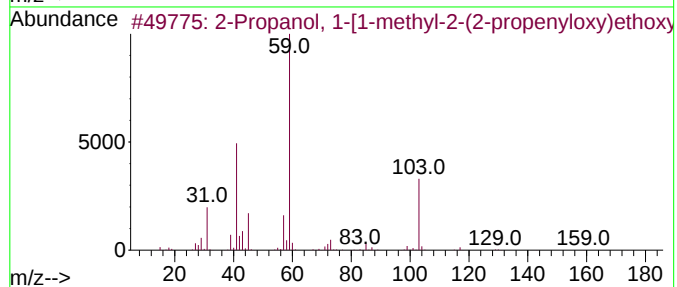
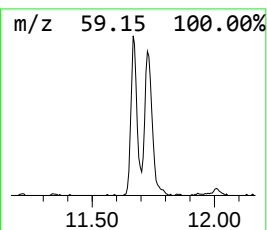
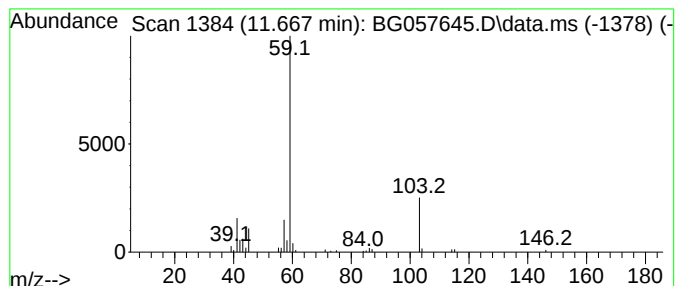
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.667	9.23 ng	90931	Naphthalene-d8	11.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	83		
2	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	74		
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72		
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	72		
5	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1010367-13-4	59		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
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Sample : 02997-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DMA-1103

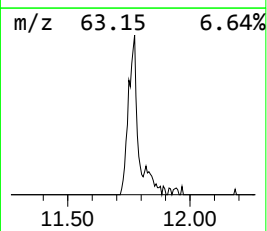
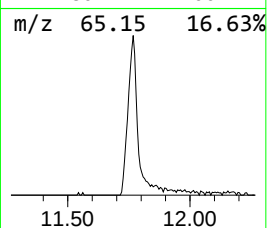
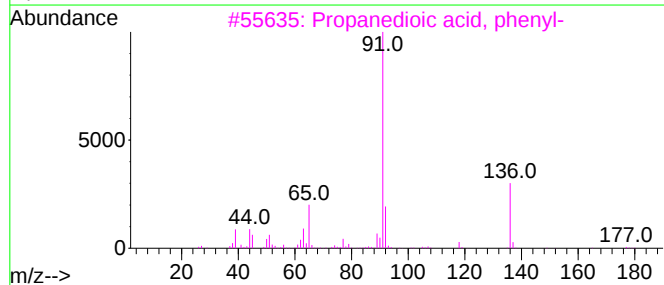
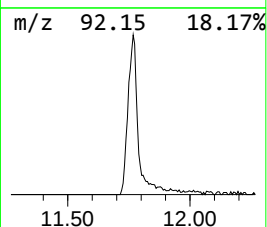
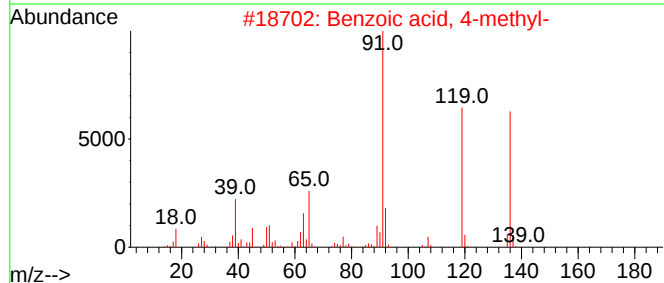
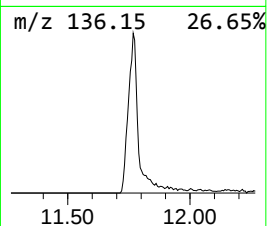
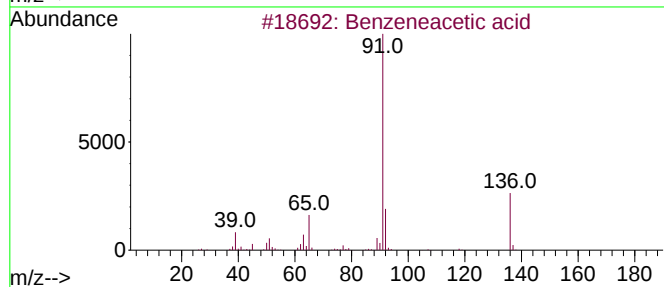
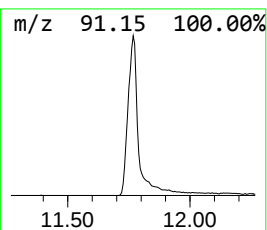
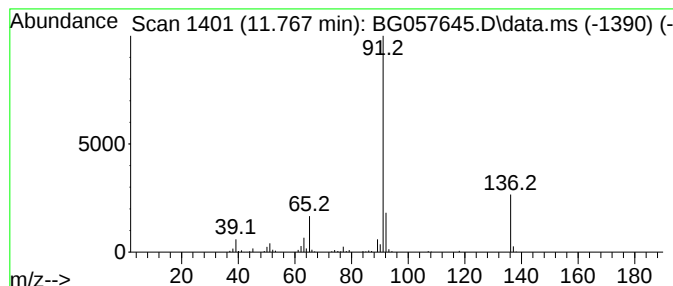
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzeneacetic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.767	46.20 ng	455198	Naphthalene-d8	11.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	95
2			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	59
3			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	59
4			Benzene, (iodomethyl)-	218	C7H7I	000620-05-3	53
5			Benzeneacetaldehyde	120	C8H8O	000122-78-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
Operator : CG/JU
Sample : 02997-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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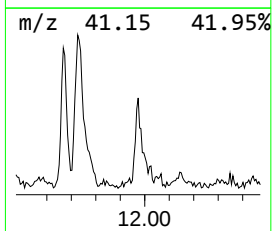
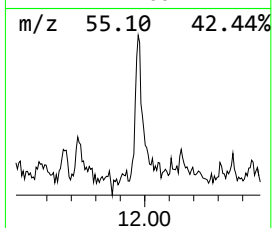
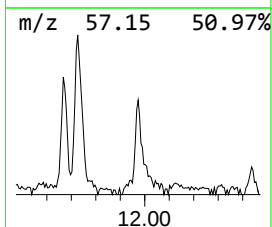
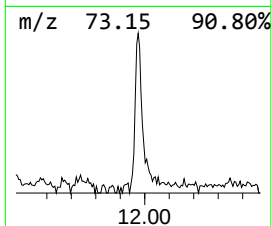
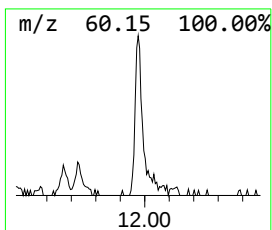
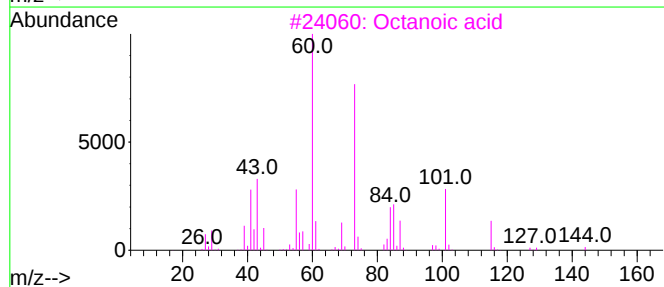
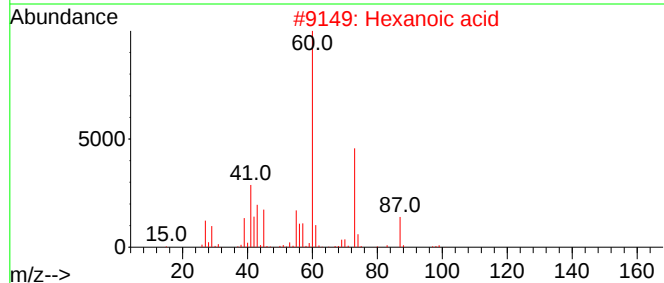
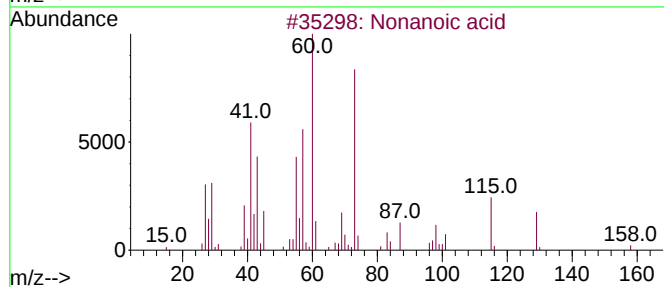
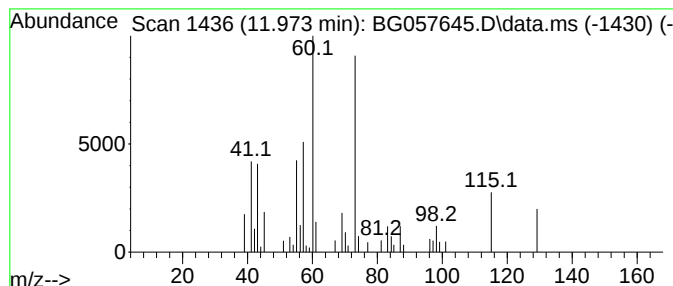
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Nonanoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.973	7.06 ng	69528	Naphthalene-d8	11.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	90
2			Hexanoic acid	116	C6H12O2	000142-62-1	50
3			Octanoic acid	144	C8H16O2	000124-07-2	42
4			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	38
5			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
Operator : CG/JU
Sample : 02997-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DMA-1103

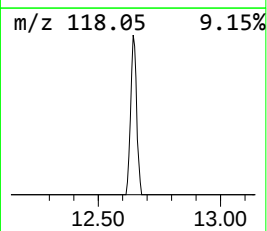
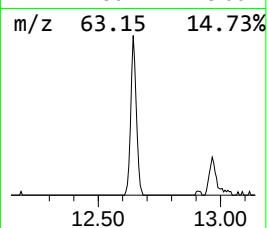
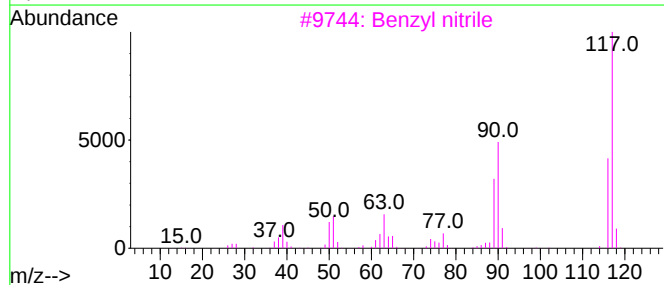
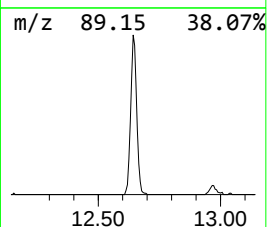
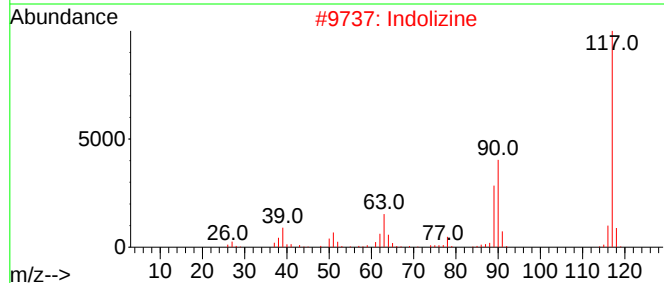
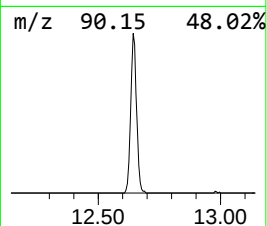
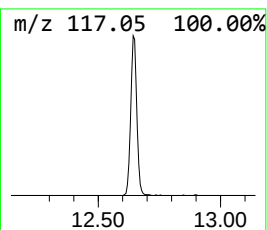
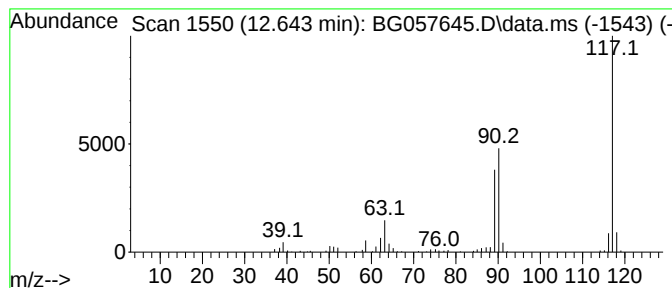
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Indole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.643	25.00 ng	246341	Naphthalene-d8	11.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	97
2			Indolizine	117	C8H7N	000274-40-8	90
3			Benzyl nitrile	117	C8H7N	000140-29-4	87
4			Benzene, 1-isocyano-2-methyl-	117	C8H7N	010468-64-1	87
5			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
Operator : CG/JU
Sample : 02997-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DMA-1103

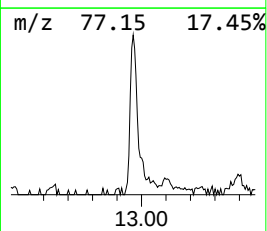
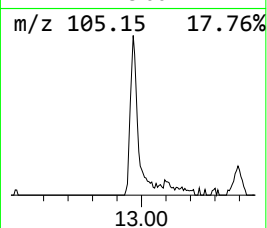
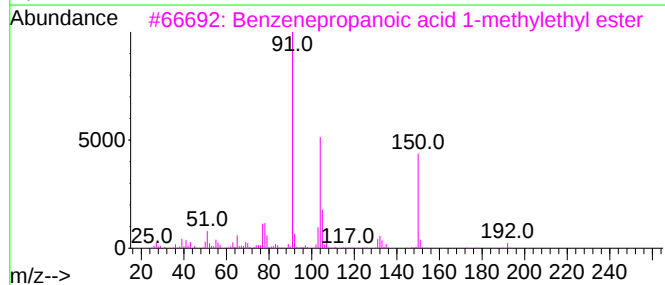
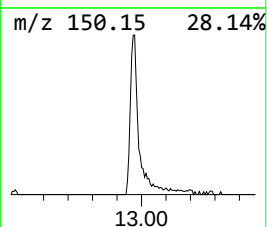
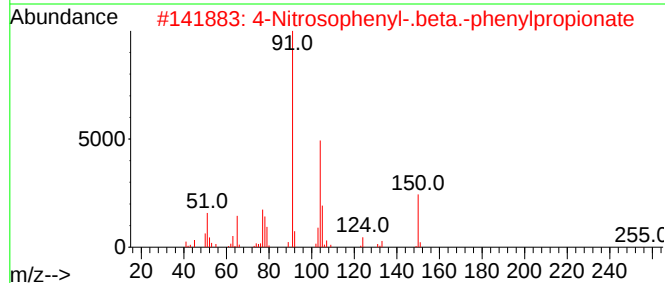
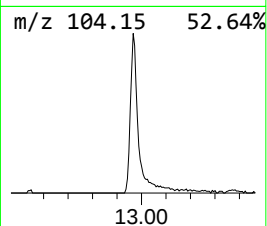
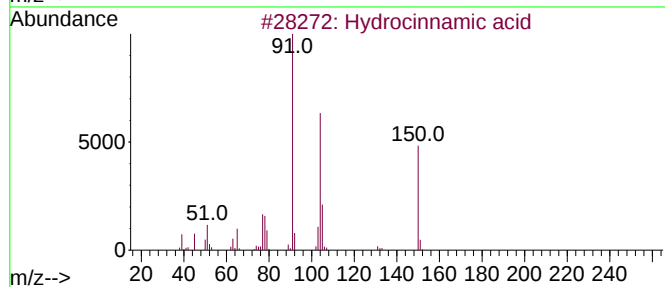
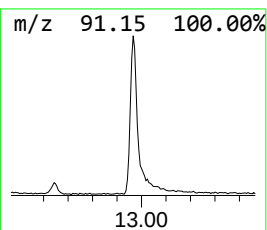
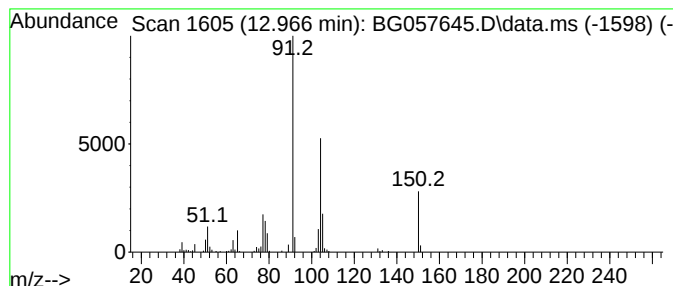
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Hydrocinnamic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.966	22.96 ng	226209	Naphthalene-d8	11.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrocinnamic acid	150	C9H10O2	000501-52-0	97
2			4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	86
3			Benzenepropanoic acid 1-methylet...	192	C12H16O2	022767-95-9	78
4			Benzenepropanoic acid, silver(1+...	256	C9H9AgO2	075112-79-7	53
5			Acetic acid, trifluoro-, 2-pheny...	218	C10H9F3O2	055419-66-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
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Sample : 02997-01
Misc :
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Instrument :
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ClientSampleId :
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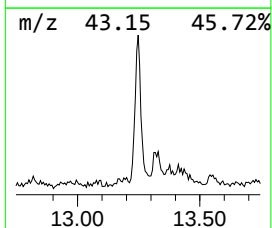
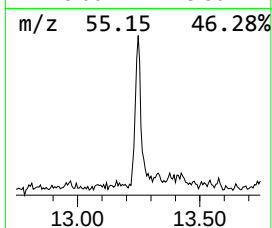
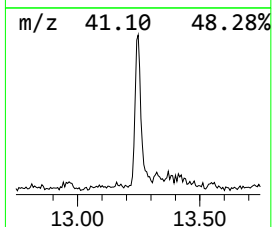
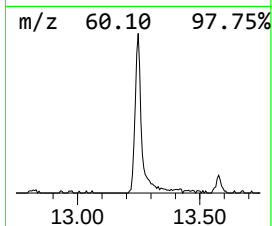
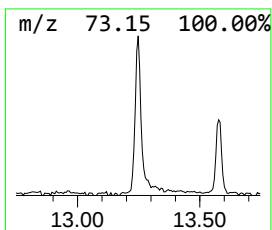
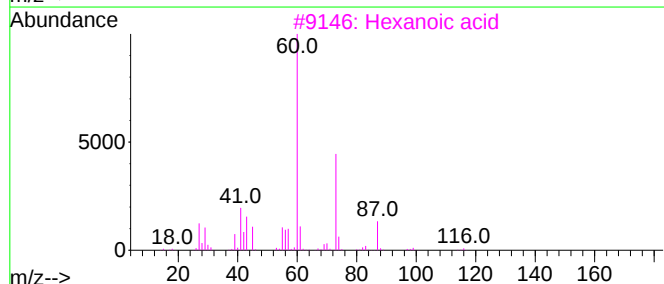
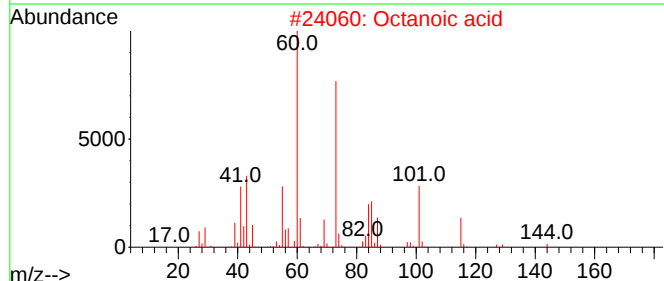
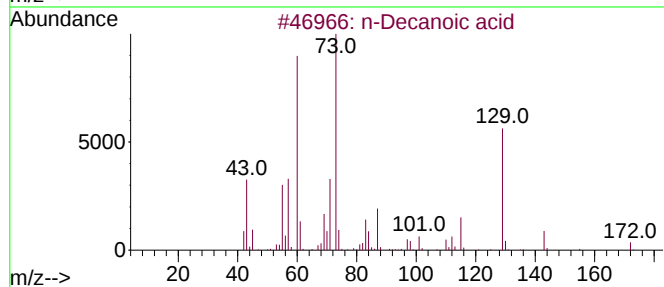
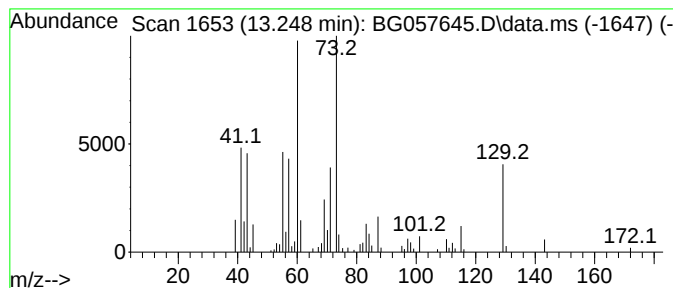
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 n-Decanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.248	10.91 ng	168707	Acenaphthene-d10	14.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	97
2			Octanoic acid	144	C8H16O2	000124-07-2	47
3			Hexanoic acid	116	C6H12O2	000142-62-1	43
4			Heptanoic acid	130	C7H14O2	000111-14-8	43
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
Operator : CG/JU
Sample : 02997-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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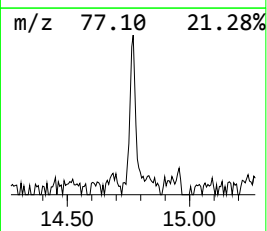
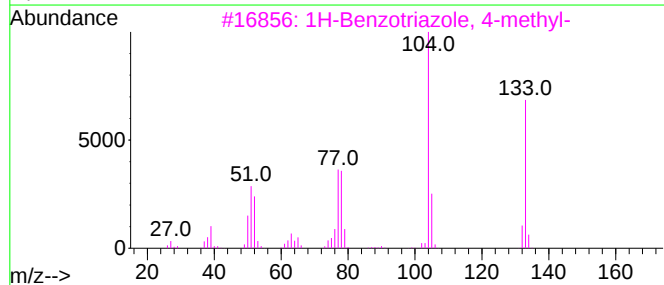
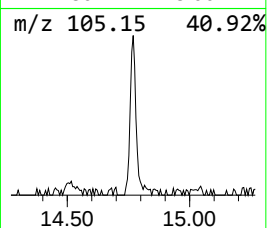
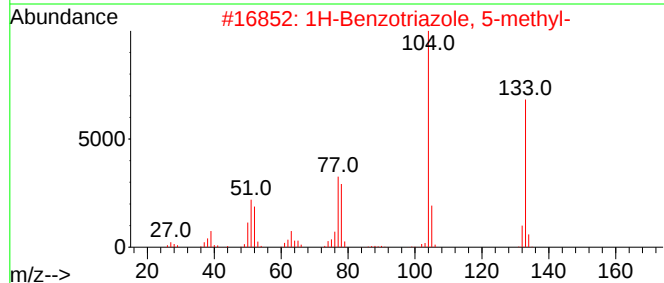
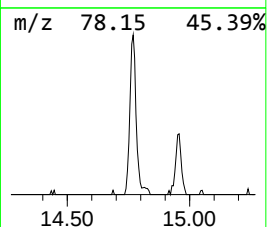
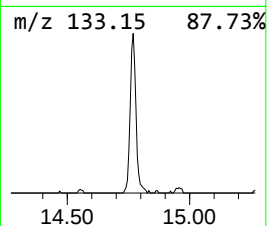
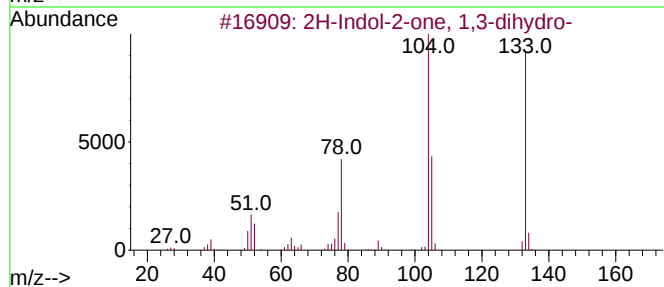
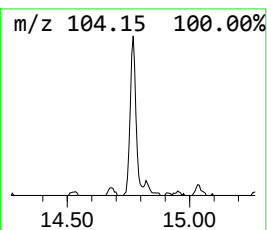
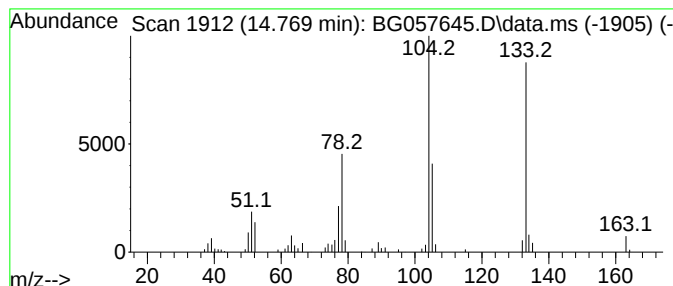
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 2H-Indol-2-one, 1,3-dihydro- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.769	6.64 ng	102646	Acenaphthene-d10	14.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	96
2			1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	87
3			1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	87
4			Benzene, 1-isocyanato-2-methyl-	133	C8H7NO	000614-68-6	83
5			Benzene, 1-isocyanato-3-methyl-	133	C8H7NO	000621-29-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
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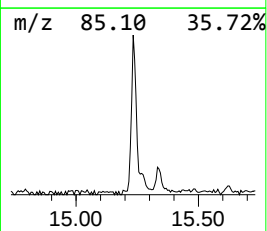
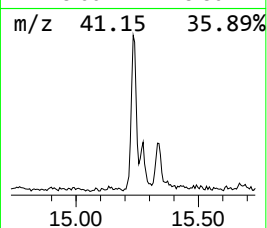
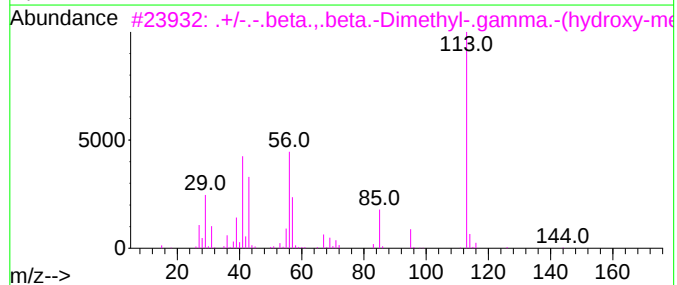
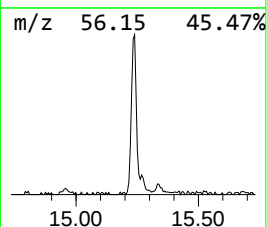
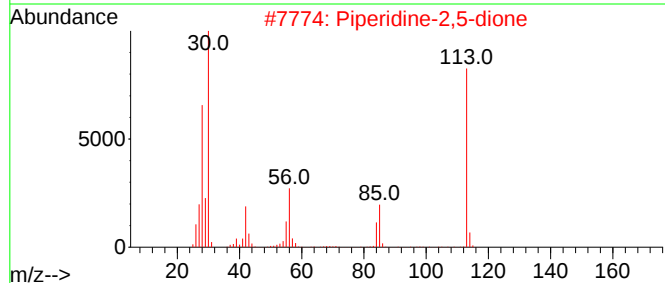
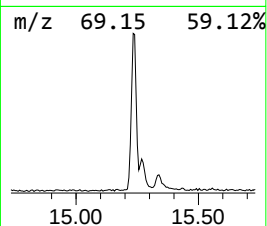
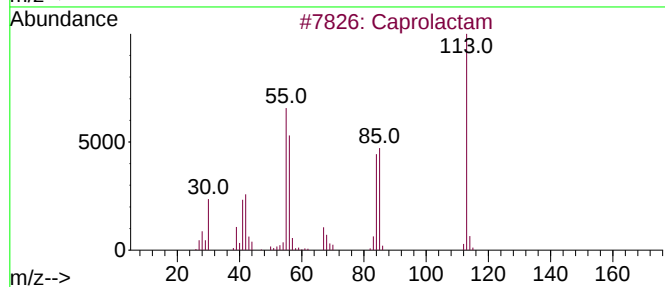
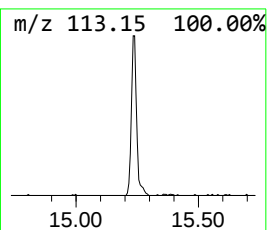
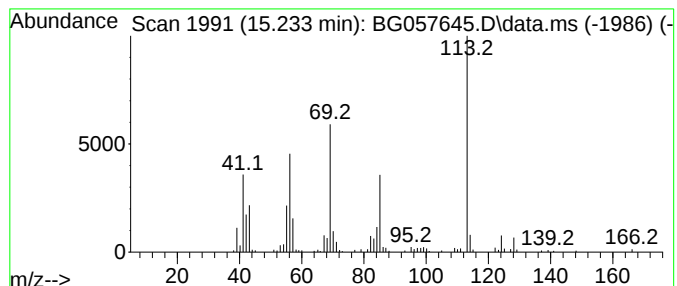
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Piperidine-2,5-dione Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	14.11 ng	218283	Acenaphthene-d10	14.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caprolactam	113	C6H11NO	000105-60-2	68
2			Piperidine-2,5-dione	113	C5H7NO2	052065-78-8	59
3			.+/--.beta.,.beta.-Dimethyl-.ga...	144	C7H12O3	052398-48-8	59
4			2H-Pyrrol-2-one, 1,5-dihydro-4-m...	113	C5H7NO2	069778-83-2	50
5			1-(3-methoxyphenyl)-2-(piperazin...	248	C14H20N2O2	1000455-99-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
Operator : CG/JU
Sample : 02997-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DMA-1103

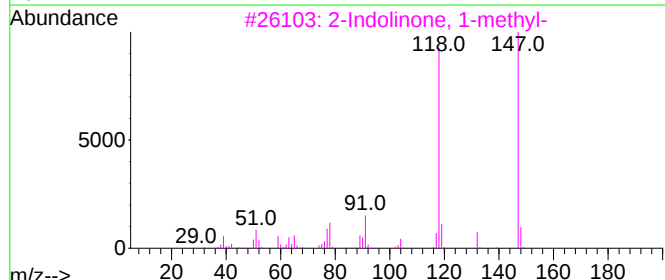
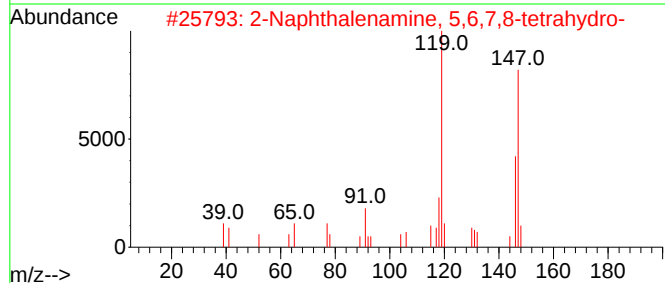
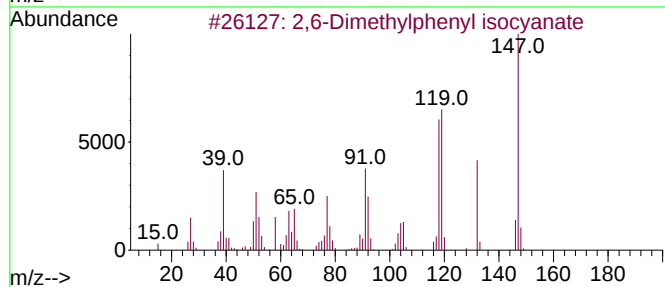
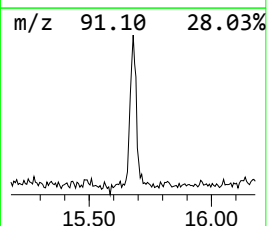
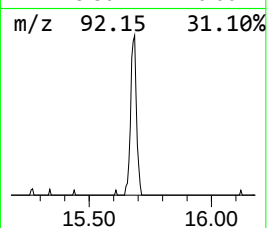
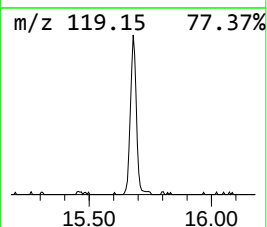
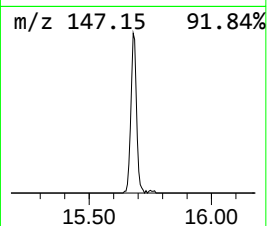
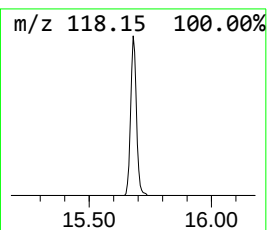
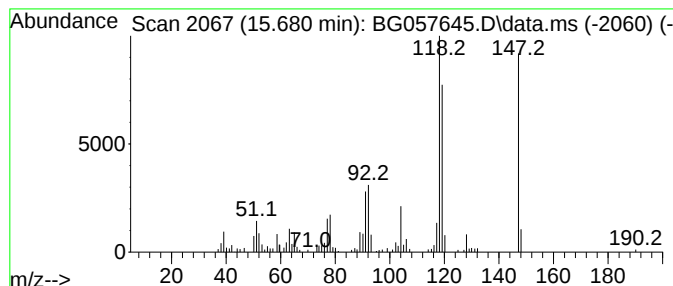
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 2,6-Dimethylphenyl isocyanate Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.680	10.80 ng	167029	Acenaphthene-d10	14.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Dimethylphenyl isocyanate	147	C9H9NO	028556-81-2	86
2			2-Naphthalenamine, 5,6,7,8-tetra...	147	C10H13N	002217-43-8	70
3			2-Indolinone, 1-methyl-	147	C9H9NO	000061-70-1	64
4			1H-Indole-1-carboxaldehyde, 2,3-...	147	C9H9NO	002861-59-8	60
5			(2-Benzimidazolyl)methylamine	147	C8H9N3	005805-57-2	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
Operator : CG/JU
Sample : 02997-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DMA-1103

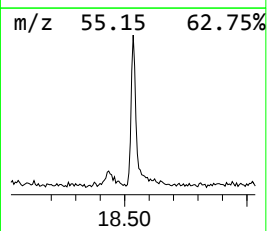
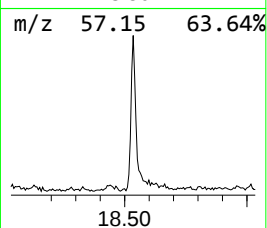
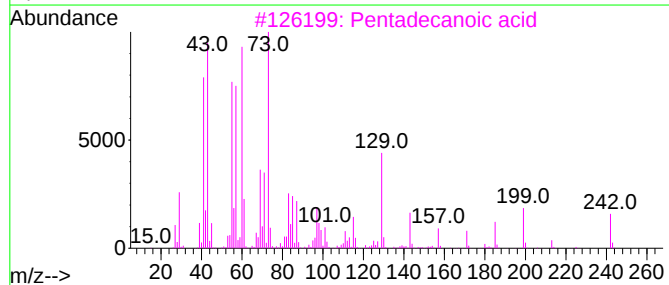
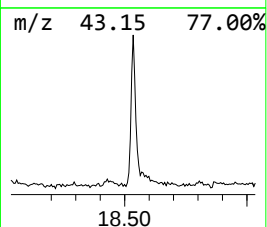
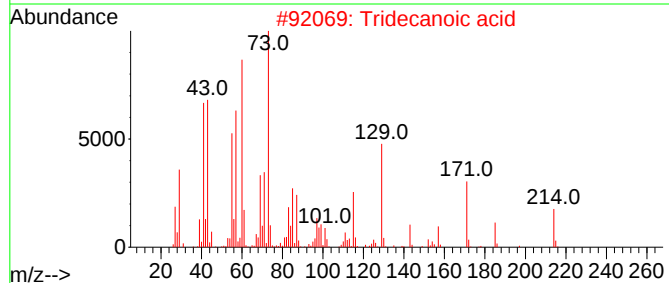
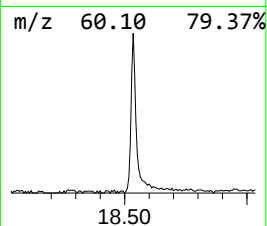
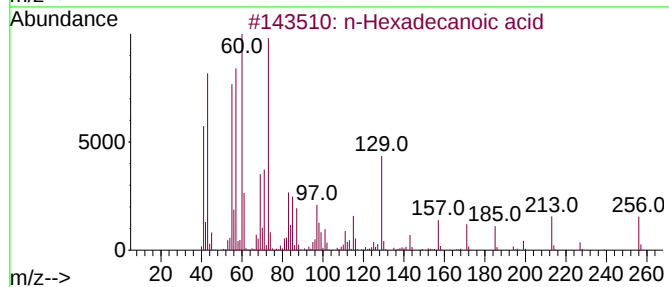
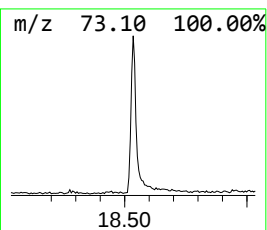
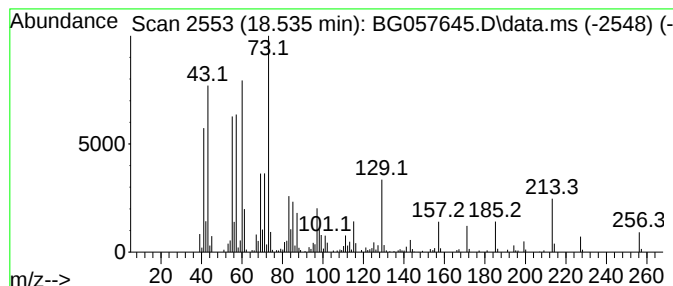
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.535	15.90 ng	316718	Phenanthrene-d10	17.695

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	92
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
Data File : BG057645.D
Acq On : 6 Jun 2023 20:16
Operator : CG/JU
Sample : 02997-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DMA-1103

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.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,...	3.990	11.8	ng	69877	1	8.337	118562	20.0
Butanoic acid	4.360	10.6	ng	62673	1	8.337	118562	20.0
Butanoic acid, ...	5.241	57.4	ng	340099	1	8.337	118562	20.0
Butanoic acid, ...	5.394	32.2	ng	190717	1	8.337	118562	20.0
2-Heptanol	6.281	13.2	ng	78185	1	8.337	118562	20.0
Pentanoic acid,...	6.774	28.7	ng	170310	1	8.337	118562	20.0
Heptanoic acid	8.971	21.9	ng	129870	1	8.337	118562	20.0
Hexanoic acid, ...	9.658	15.8	ng	93718	1	8.337	118562	20.0
Octanoic acid	10.557	67.2	ng	661762	2	11.174	197076	20.0
2-Propanol, 1-[...	11.667	9.2	ng	90931	2	11.174	197076	20.0
Benzeneacetic acid	11.767	46.2	ng	455198	2	11.174	197076	20.0
Nonanoic acid	11.973	7.1	ng	69528	2	11.174	197076	20.0
Indole	12.643	25.0	ng	246341	2	11.174	197076	20.0
Hydrocinnamic acid	12.966	23.0	ng	226209	2	11.174	197076	20.0
n-Decanoic acid	13.248	10.9	ng	168707	3	14.957	309393	20.0
2H-Indol-2-one,...	14.769	6.6	ng	102646	3	14.957	309393	20.0
Piperidine-2,5-...	15.233	14.1	ng	218283	3	14.957	309393	20.0
2,6-Dimethylphe...	15.680	10.8	ng	167029	3	14.957	309393	20.0
n-Hexadecanoic ...	18.535	15.9	ng	316718	4	17.695	398455	20.0