

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
 Data File : BG058555.D
 Acq On : 1 Aug 2023 9:53
 Operator : MA/JU
 Sample : 03771-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PATERSON-GSMP-COMP

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-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058555.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.155	3	11	23	rBV2	1114108	2957382	7.39%	2.709%
2	3.931	125	143	148	rBV2	676056	2688869	6.72%	2.463%
3	4.195	167	188	191	rBV3	378857	1603287	4.00%	1.469%
4	4.847	294	299	304	rBV	243557	518099	1.29%	0.475%
5	5.341	378	383	389	rBV	280367	552870	1.38%	0.507%
6	5.399	389	393	403	rVB	386943	611882	1.53%	0.561%
7	7.009	597	667	669	rBV5	1731776	19722310	49.26%	18.068%
8	7.820	742	805	810	rBV4	2973173	40035876	100.00%	36.678%
9	8.372	864	899	901	rBV2	1293756	8612112	21.51%	7.890%
10	8.637	932	944	950	rBV	2447806	5845720	14.60%	5.355%
11	8.854	950	981	984	rVB	1022845	6165008	15.40%	5.648%
12	8.983	996	1003	1014	rBV	495033	931397	2.33%	0.853%
13	9.483	1069	1088	1094	rBV2	311456	1180689	2.95%	1.082%
14	10.088	1171	1191	1198	rBV4	385050	1420121	3.55%	1.301%
15	10.623	1275	1282	1291	rVB	286503	544573	1.36%	0.499%
16	11.304	1376	1398	1403	rBV	604644	2598238	6.49%	2.380%
17	12.133	1532	1539	1549	rVB	566835	1020014	2.55%	0.934%
18	12.503	1592	1602	1617	rVB	387986	1019116	2.55%	0.934%
19	12.797	1644	1652	1662	rBV	288583	581687	1.45%	0.533%
20	13.085	1695	1701	1711	rVB	1247228	1991359	4.97%	1.824%
21	13.361	1743	1748	1755	rVB	446113	702751	1.76%	0.644%
22	14.295	1900	1907	1913	rBV	278466	499300	1.25%	0.457%
23	14.465	1926	1936	1944	rVB2	488679	915119	2.29%	0.838%
24	15.952	2183	2189	2194	rBV	1006439	1530524	3.82%	1.402%
25	17.209	2398	2403	2408	rBV	536863	791839	1.98%	0.725%
26	19.824	2843	2848	2856	rVB	1764842	2289299	5.72%	2.097%
27	21.445	3119	3124	3133	rVB2	531209	832195	2.08%	0.762%
28	24.518	3637	3647	3660	rVB2	359434	992555	2.48%	0.909%

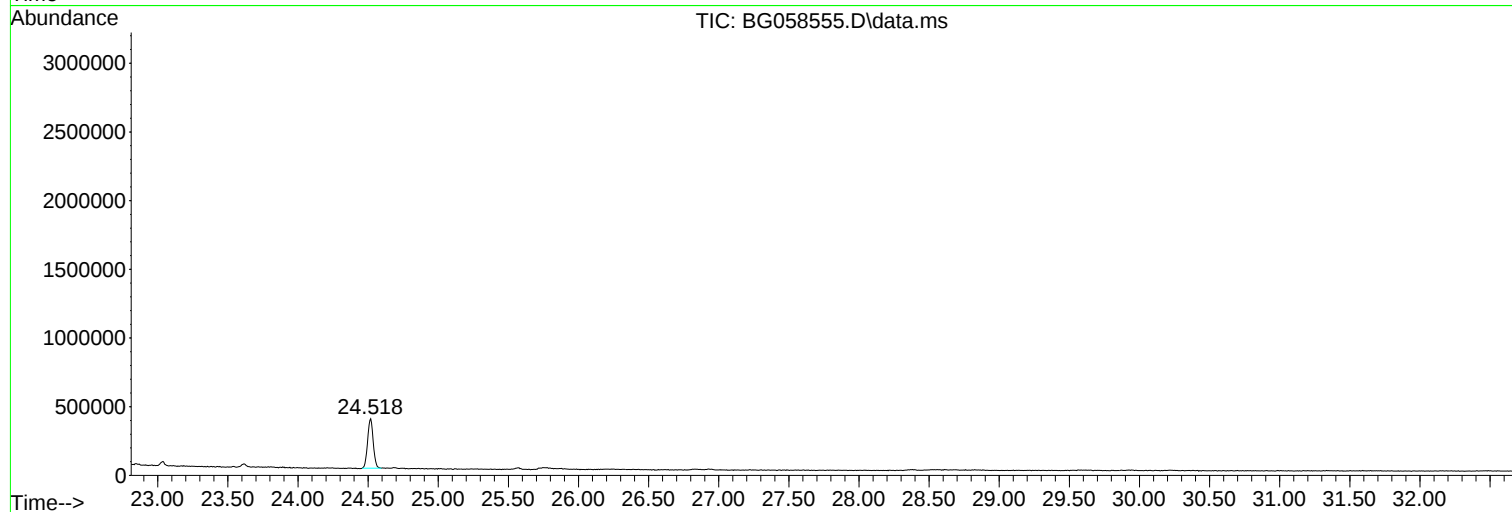
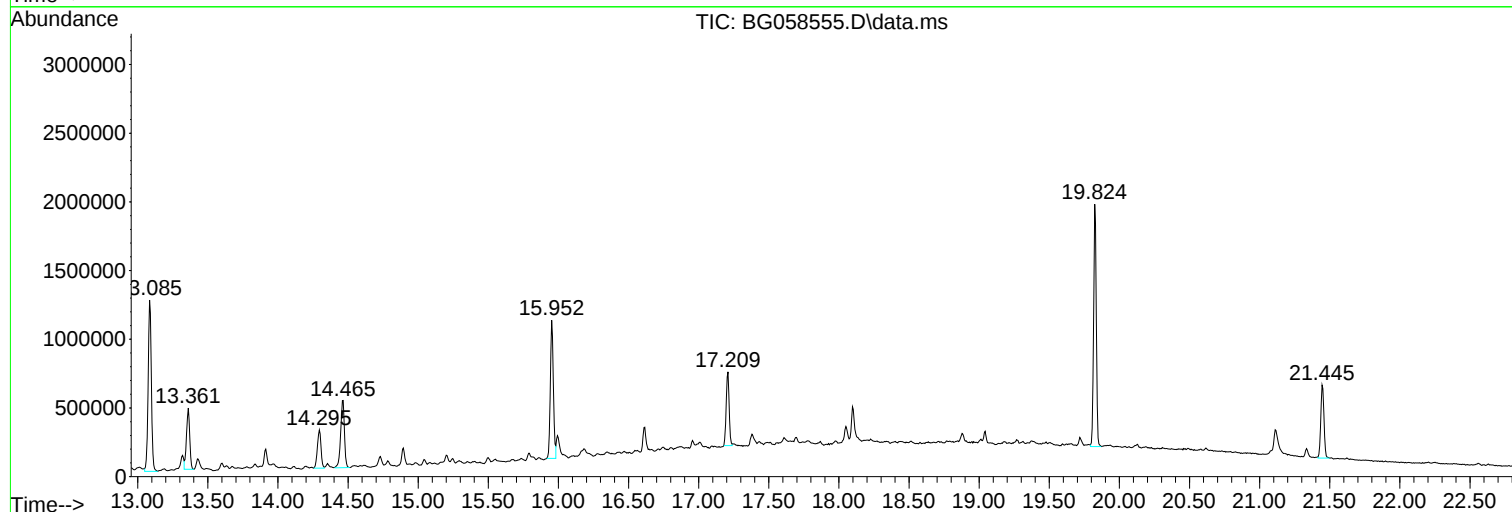
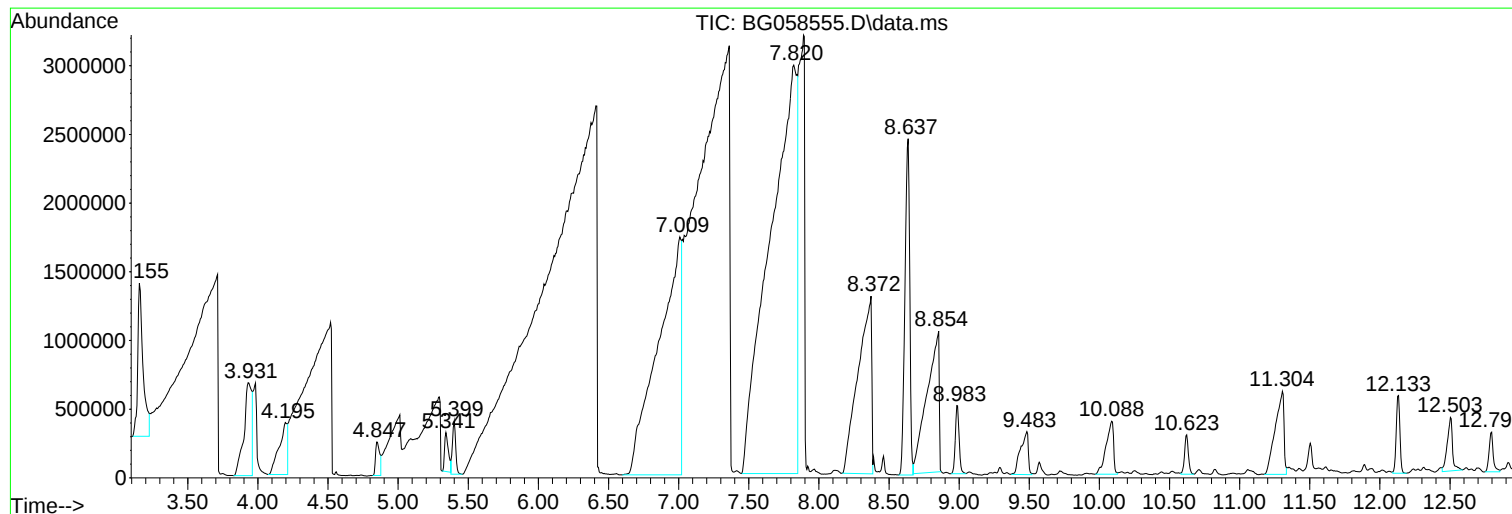
Sum of corrected areas: 109154191

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058555.D
Acq On : 1 Aug 2023 9:53
Operator : MA/JU
Sample : 03771-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PATERSON-GSMP-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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\BG080123\
Data File : BG058555.D
Acq On : 1 Aug 2023 9:53
Operator : MA/JU
Sample : 03771-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PATERSON-GSMP-COMP

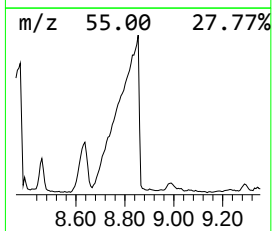
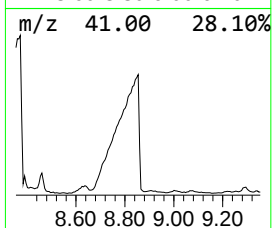
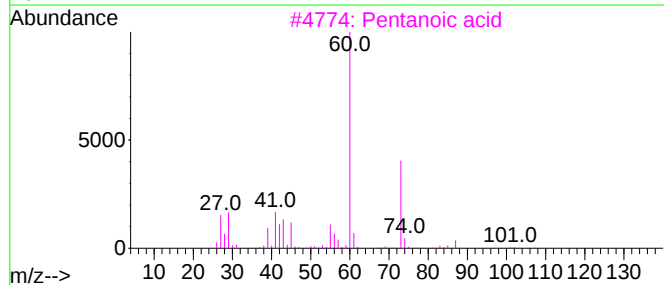
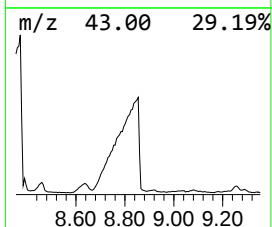
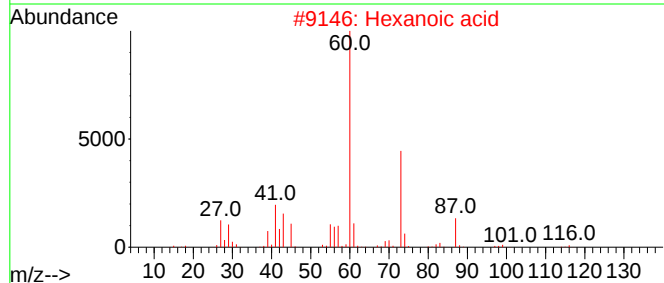
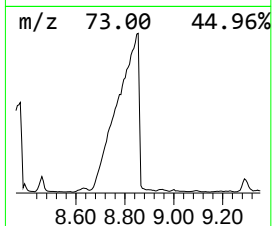
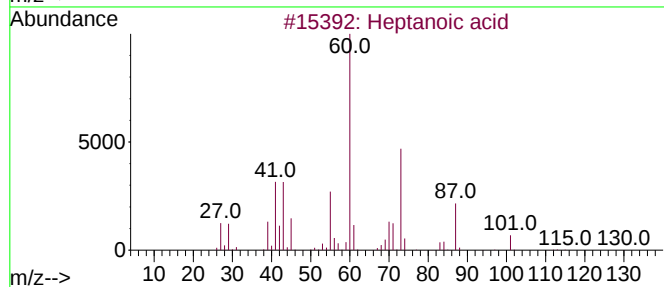
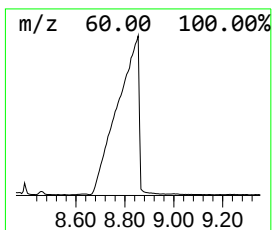
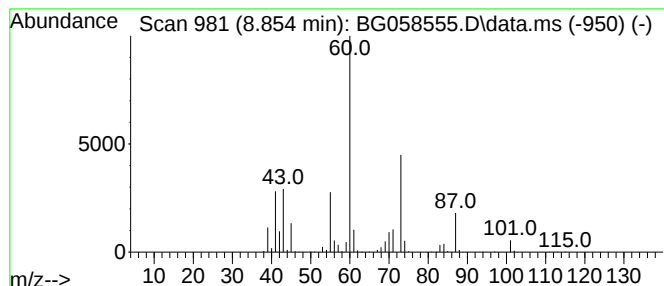
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Heptanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.854	3.08 ng	6165010	1,4-Dichlorobenzene-d4	7.814

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			Pentanoic acid	102	C5H10O2	000109-52-4	64
4			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058555.D
Acq On : 1 Aug 2023 9:53
Operator : MA/JU
Sample : 03771-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PATERSON-GSMP-COMP

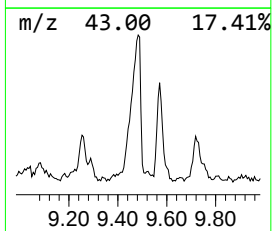
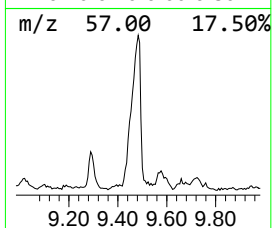
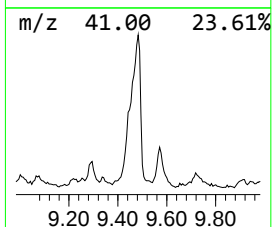
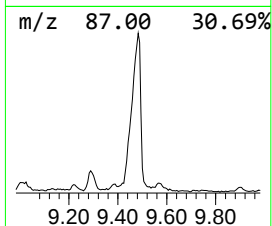
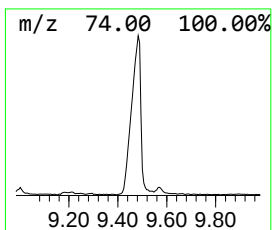
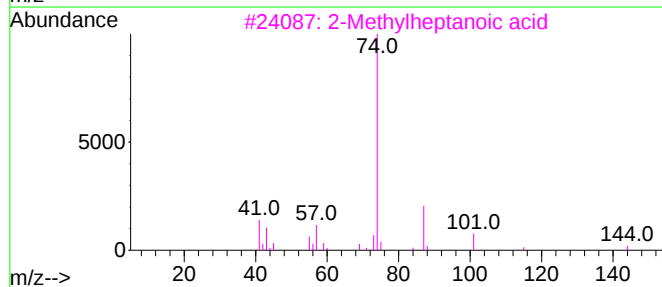
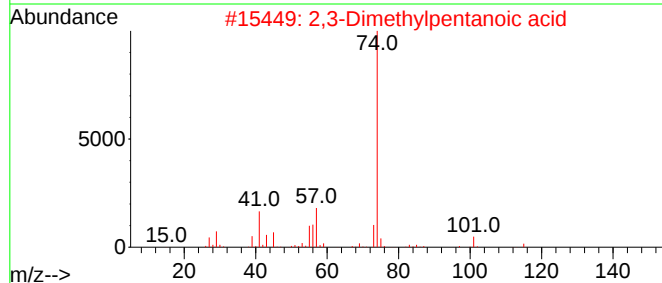
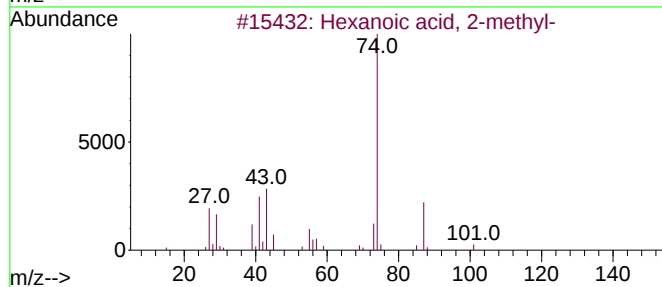
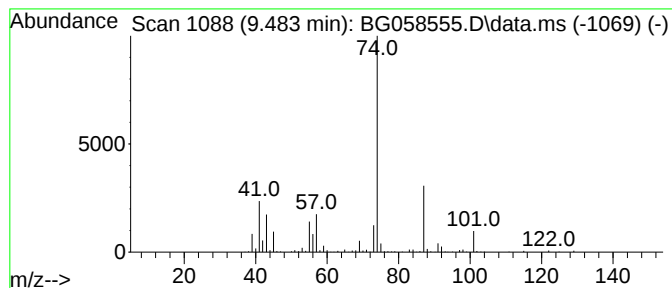
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexanoic acid, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.483	43.36 ng	1180690	Naphthalene-d8	10.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72
2			2,3-Dimethylpentanoic acid	130	C7H14O2	082608-03-5	59
3			2-Methylheptanoic acid	144	C8H16O2	001188-02-9	59
4			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	53
5			Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058555.D
Acq On : 1 Aug 2023 9:53
Operator : MA/JU
Sample : 03771-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PATERSON-GSMP-COMP

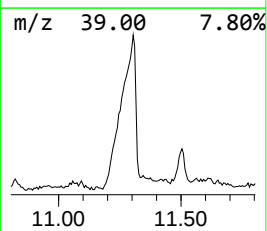
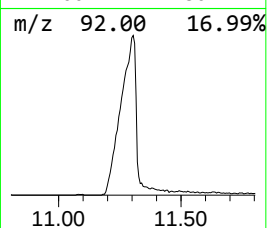
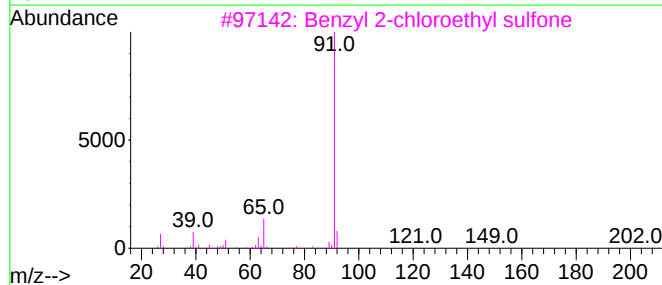
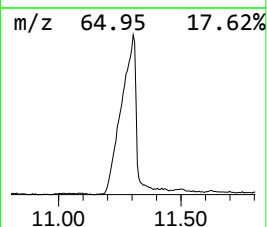
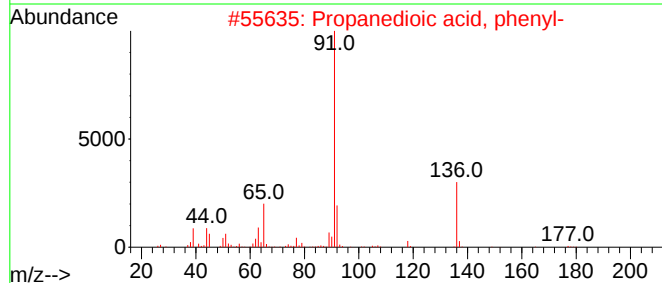
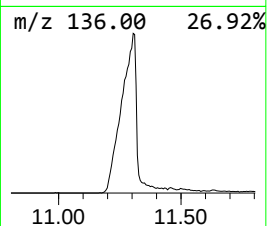
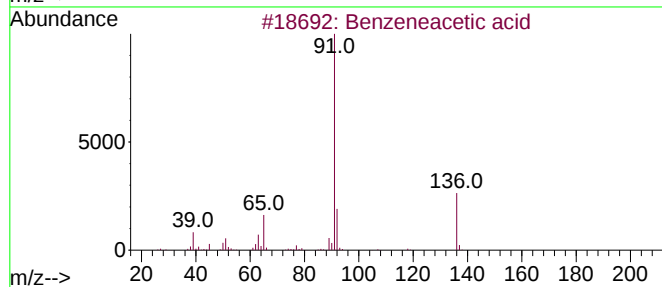
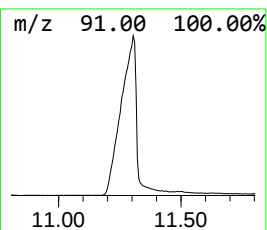
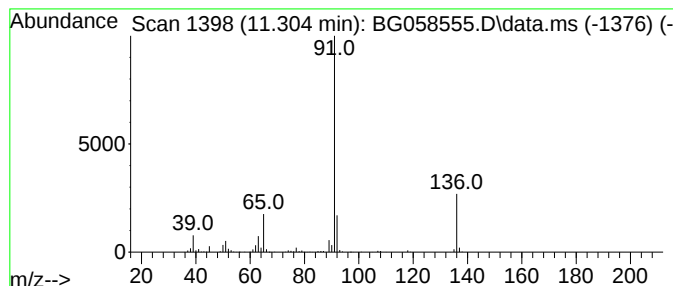
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzeneacetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.304	95.42 ng	2598240	Naphthalene-d8	10.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	95
2			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	78
3			Benzyl 2-chloroethyl sulfone	218	C9H11ClO2S	066998-67-2	50
4			Benzeneacetamide	135	C8H9NO	000103-81-1	43
5			Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058555.D
Acq On : 1 Aug 2023 9:53
Operator : MA/JU
Sample : 03771-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PATERSON-GSMP-COMP

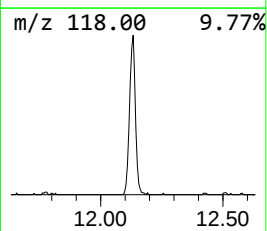
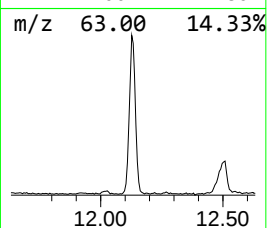
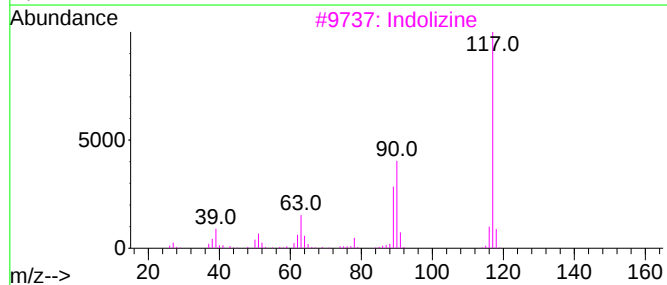
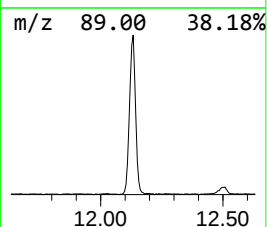
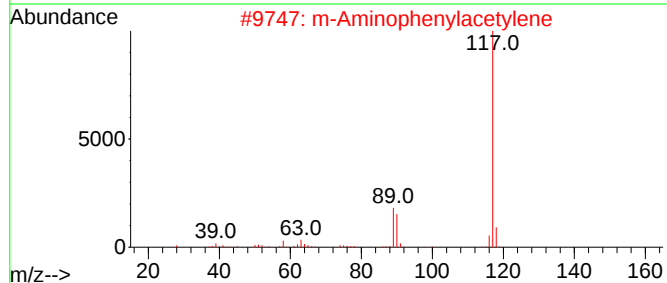
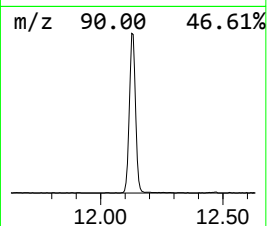
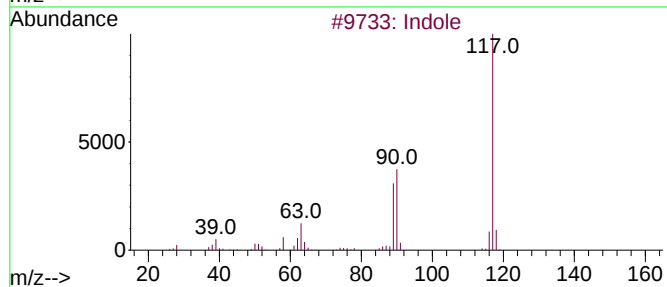
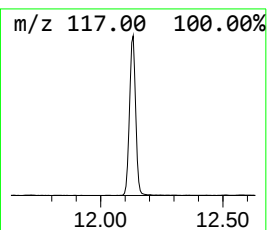
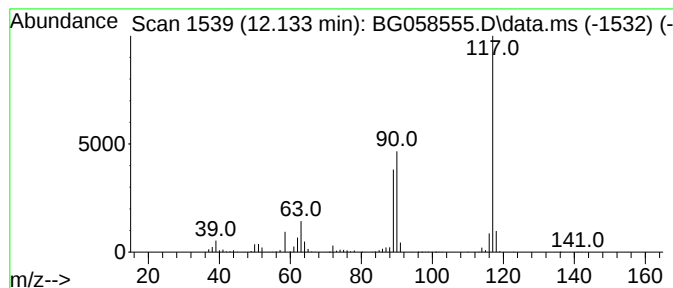
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Indole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.133	37.46 ng	1020010	Naphthalene-d8	10.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	97
2			m-Aminophenylacetylene	117	C8H7N	054060-30-9	91
3			Indolizine	117	C8H7N	000274-40-8	90
4			Benzene, 1-isocyano-2-methyl-	117	C8H7N	010468-64-1	87
5			Benzyl nitrile	117	C8H7N	000140-29-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058555.D
Acq On : 1 Aug 2023 9:53
Operator : MA/JU
Sample : 03771-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PATERSON-GSMP-COMP

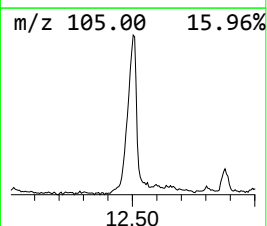
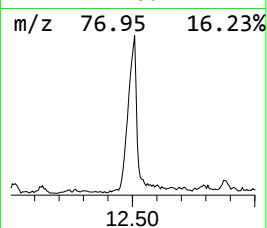
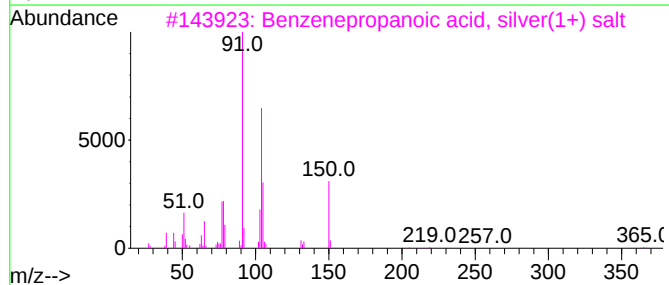
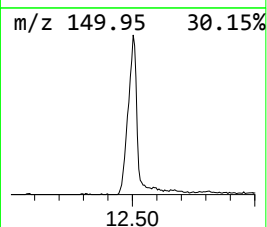
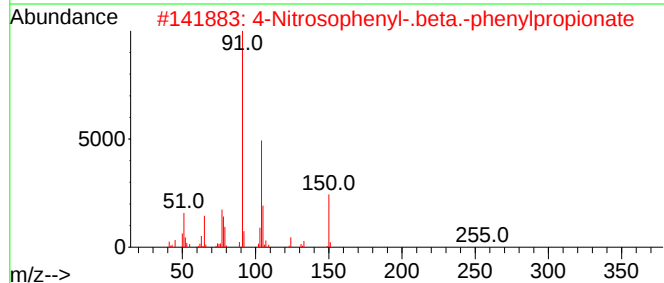
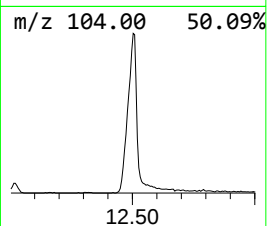
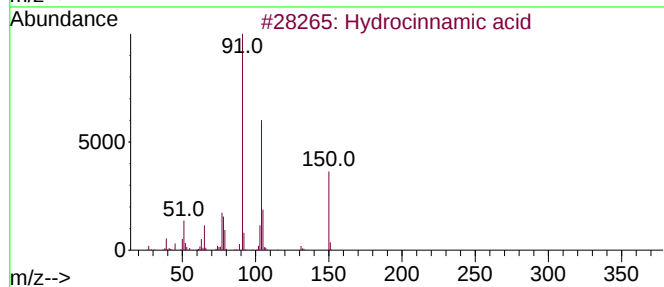
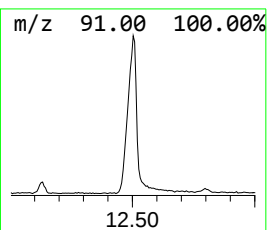
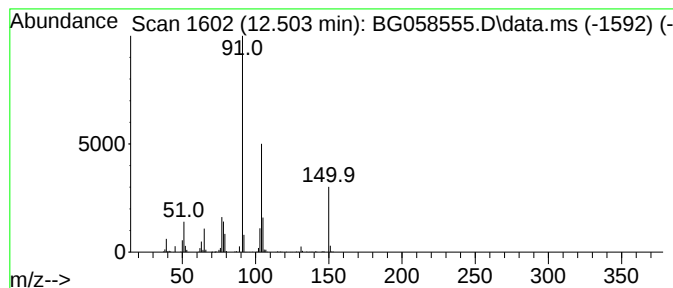
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hydrocinnamic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.503	37.43 ng	1019120	Naphthalene-d8	10.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrocinnamic acid	150	C9H10O2	000501-52-0	96
2			4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	86
3			Benzenepropanoic acid, silver(1+...	256	C9H9AgO2	075112-79-7	80
4			Pentafluoropropionic acid, 2-phe...	268	C11H9F5O2	081089-48-7	59
5			Acetic acid, trifluoro-, 2-pheny...	218	C10H9F3O2	055419-66-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058555.D
Acq On : 1 Aug 2023 9:53
Operator : MA/JU
Sample : 03771-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

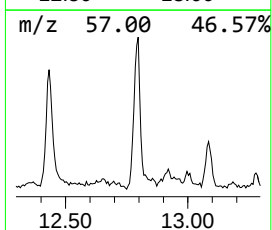
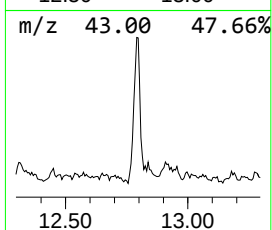
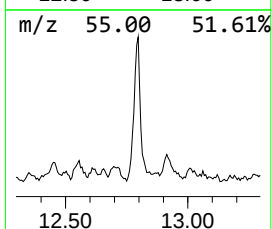
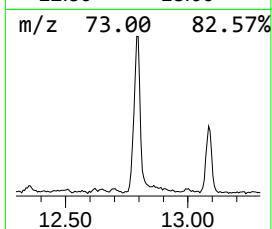
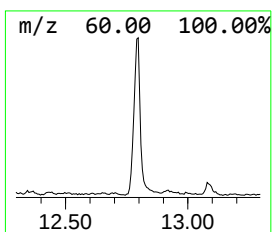
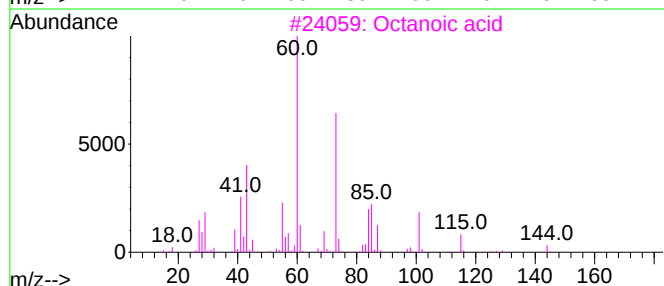
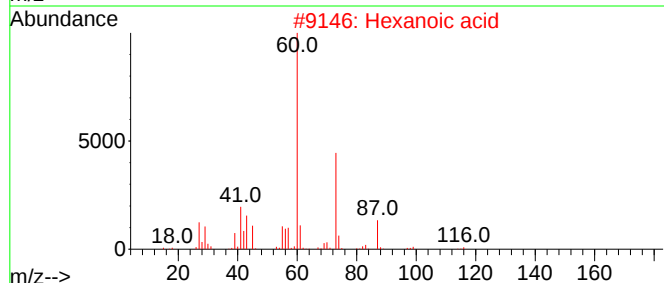
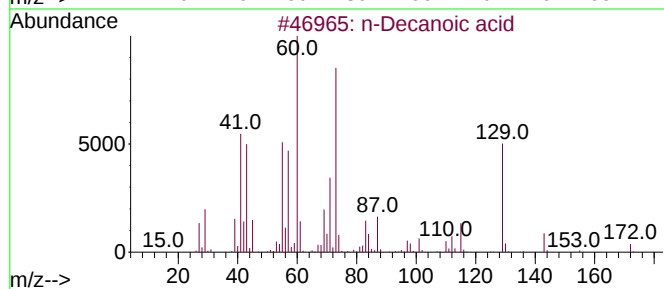
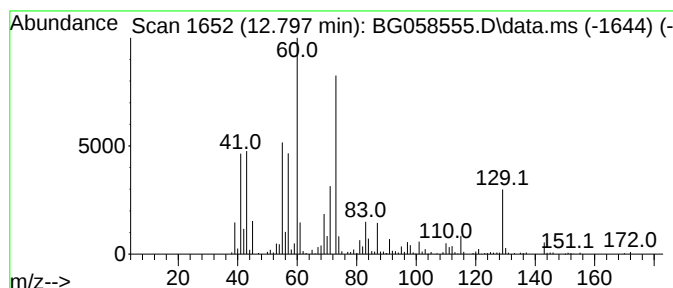
Instrument :
BNA_G
ClientSampleId :
PATERSON-GSMP-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Decanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.797	12.71 ng	581687	Acenaphthene-d10	14.465	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	97
2	Hexanoic acid	116	C6H12O2	000142-62-1	52
3	Octanoic acid	144	C8H16O2	000124-07-2	50
4	Heptanoic acid	130	C7H14O2	000111-14-8	50
5	Nonanoic acid	158	C9H18O2	000112-05-0	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058555.D
Acq On : 1 Aug 2023 9:53
Operator : MA/JU
Sample : 03771-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

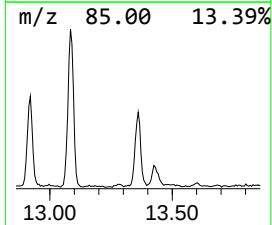
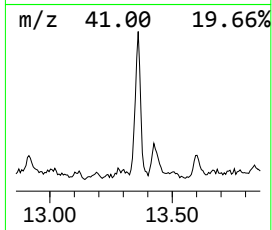
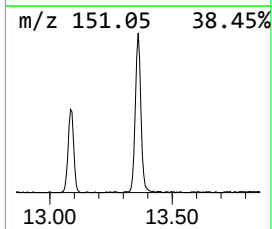
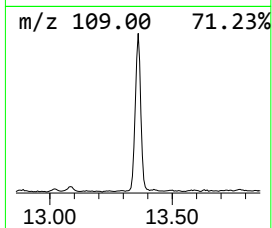
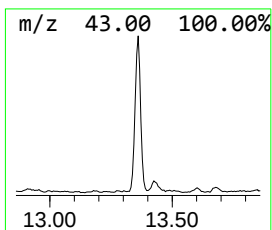
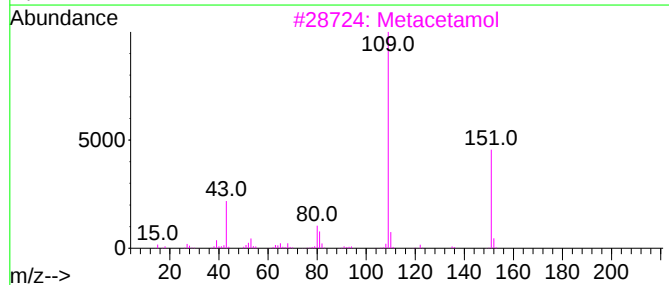
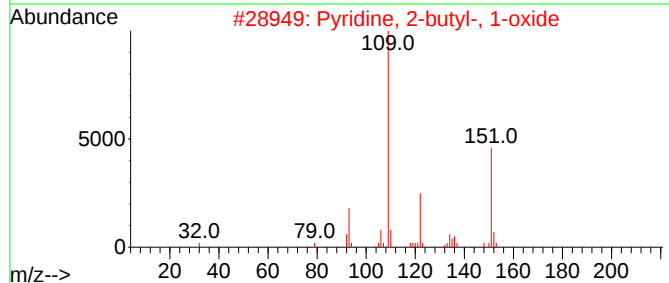
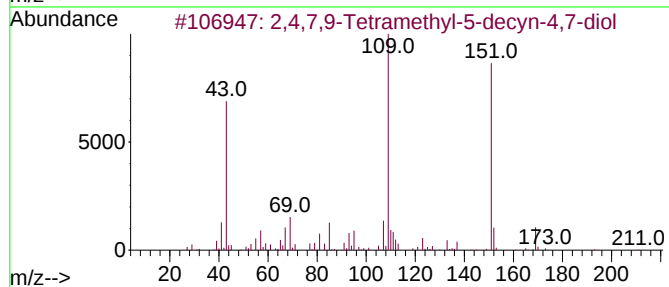
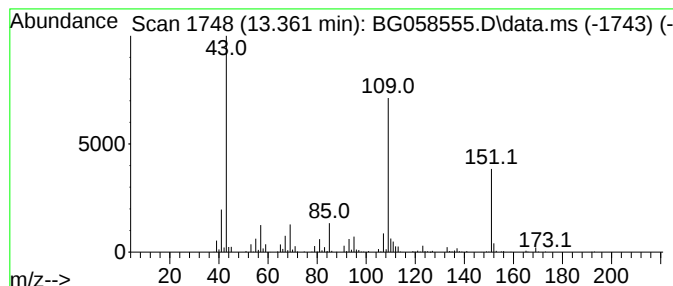
Instrument :
BNA_G
ClientSampleId :
PATERSON-GSMP-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.361	15.36 ng	702751	Acenaphthene-d10		14.465	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	59
3	Metacetamol		151	C8H9NO2	000621-42-1	58
4	p-Isopropoxyaniline		151	C9H13NO	007664-66-6	58
5	N-(4-tert-Butoxyphenyl)acetamide		207	C12H17NO2	002109-73-1	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058555.D
Acq On : 1 Aug 2023 9:53
Operator : MA/JU
Sample : 03771-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

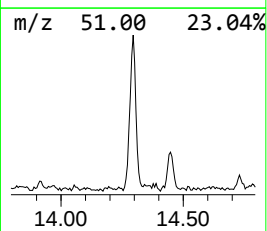
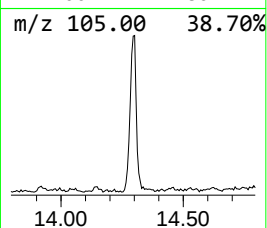
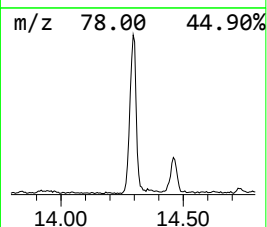
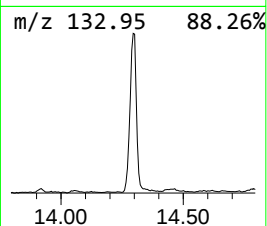
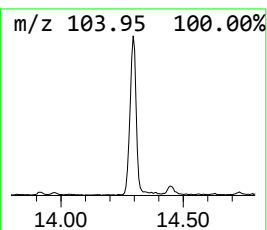
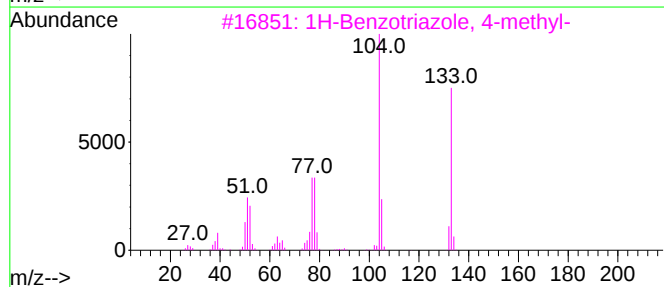
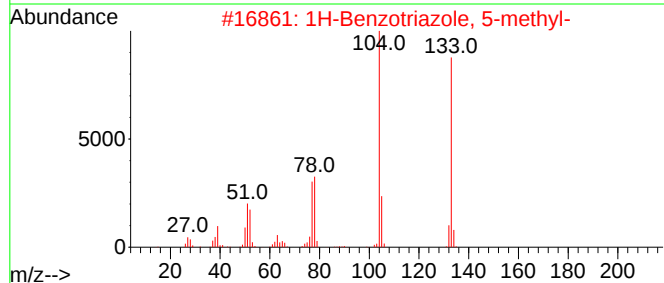
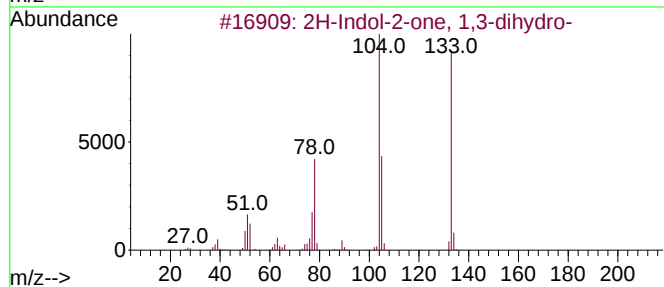
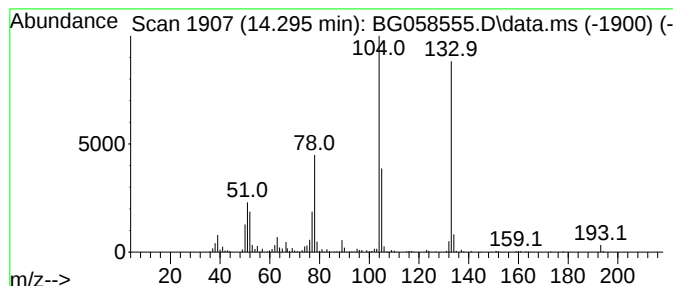
Instrument :
BNA_G
ClientSampleId :
PATERSON-GSMP-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2H-Indol-2-one, 1,3-dihydro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.295	10.91 ng	499300	Acenaphthene-d10	14.465	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	95
2	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	94
3	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	91
4	Benzene, 1-isocyanato-3-methyl-	133	C8H7NO	000621-29-4	87
5	1H-Indole, 2,3-dihydro-4-methyl-	133	C9H11N	062108-16-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058555.D
Acq On : 1 Aug 2023 9:53
Operator : MA/JU
Sample : 03771-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PATERSON-GSMP-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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
Heptanoic acid	8.854	3.1	ng	6165010	1	7.814	40035900	20.0
Hexanoic acid, ...	9.483	43.4	ng	1180690	2	10.623	544573	20.0
Benzeneacetic acid	11.304	95.4	ng	2598240	2	10.623	544573	20.0
Indole	12.133	37.5	ng	1020010	2	10.623	544573	20.0
Hydrocinnamic acid	12.503	37.4	ng	1019120	2	10.623	544573	20.0
n-Decanoic acid	12.797	12.7	ng	581687	3	14.465	915119	20.0
2,4,7,9-Tetrame...	13.361	15.4	ng	702751	3	14.465	915119	20.0
2H-Indol-2-one,...	14.295	10.9	ng	499300	3	14.465	915119	20.0