

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
 Data File : BG054885.D
 Acq On : 8 Sep 2022 15:45
 Operator : CG/JU
 Sample : N4537-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW2

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-BG082522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054885.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.769	76	82	92	rBV	34177	55493	2.75%	0.419%
2	3.986	114	119	128	rBV	34795	62397	3.09%	0.471%
3	5.079	297	305	323	rBV	103854	367960	18.22%	2.780%
4	5.208	324	327	339	rVB2	12474	30602	1.52%	0.231%
5	5.690	402	409	422	rVB	203887	348375	17.25%	2.632%
6	7.000	627	632	645	rVB5	11136	27207	1.35%	0.206%
7	7.300	676	683	692	rBV	125238	244759	12.12%	1.849%
8	7.494	709	716	726	rVB2	89417	148029	7.33%	1.118%
9	7.617	731	737	750	rVB	58349	100820	4.99%	0.762%
10	8.146	820	827	833	rBV	111876	191900	9.50%	1.450%
11	8.275	844	849	854	rBV	16328	26204	1.30%	0.198%
12	8.522	883	891	897	rBV	38365	68356	3.38%	0.516%
13	8.687	914	919	933	rVB3	19075	40478	2.00%	0.306%
14	8.916	950	958	974	rBV	649569	1167083	57.78%	8.818%
15	9.327	1020	1028	1035	rBV	312018	583662	28.90%	4.410%
16	10.731	1261	1267	1275	rBV	23156	47688	2.36%	0.360%
17	10.972	1301	1308	1321	rBV	158823	307513	15.23%	2.324%
18	11.589	1404	1413	1427	rBV	119953	380552	18.84%	2.875%
19	12.083	1493	1497	1506	rVB2	21067	41554	2.06%	0.314%
20	12.347	1539	1542	1548	rVB4	14784	23061	1.14%	0.174%
21	12.682	1596	1599	1608	rVB8	13015	29688	1.47%	0.224%
22	13.240	1689	1694	1700	rVB2	35430	64942	3.22%	0.491%
23	13.293	1700	1703	1706	rBV	15811	23009	1.14%	0.174%
24	13.405	1714	1722	1729	rBV	955076	1500062	74.27%	11.334%
25	13.640	1756	1762	1773	rVB	189204	348510	17.26%	2.633%
26	13.751	1778	1781	1786	rVB4	20097	30037	1.49%	0.227%
27	13.916	1805	1809	1812	rBV4	22491	35675	1.77%	0.270%
28	14.198	1853	1857	1860	rBV2	26524	39171	1.94%	0.296%
29	14.233	1861	1863	1867	rVB2	26867	27472	1.36%	0.208%
30	14.427	1892	1896	1903	rBV8	14948	31437	1.56%	0.238%
31	14.609	1921	1927	1935	rVB7	55663	127586	6.32%	0.964%
32	14.779	1948	1956	1963	rBV2	354555	834612	41.32%	6.306%
33	15.602	2092	2096	2102	rVB3	62332	102977	5.10%	0.778%
34	16.178	2189	2194	2204	rBV	215616	475676	23.55%	3.594%
35	16.272	2205	2210	2220	rVB	709485	1149837	56.93%	8.688%
36	16.477	2243	2245	2250	rVB	42451	50976	2.52%	0.385%

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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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.801	2297	2300	2305	rBV	44345	62844	3.11%	0.475%
38	17.535	2420	2425	2430	rVB	327864	488049	24.16%	3.688%
39	17.735	2455	2459	2466	rVB2	65722	115257	5.71%	0.871%
40	20.132	2861	2867	2873	rVB	1574845	2019735	100.00%	15.261%
41	21.431	3084	3088	3097	rVB	84161	142594	7.06%	1.077%
42	21.830	3150	3156	3164	rVB2	347182	588160	29.12%	4.444%
43	25.208	3722	3731	3746	rVB3	216873	682787	33.81%	5.159%

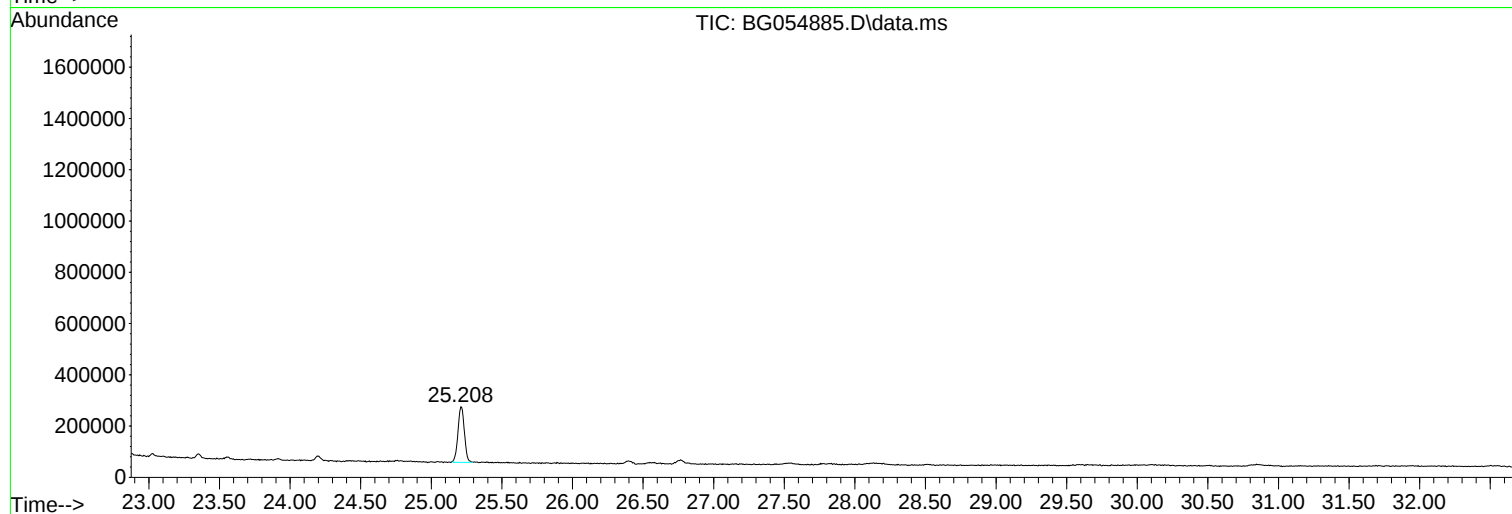
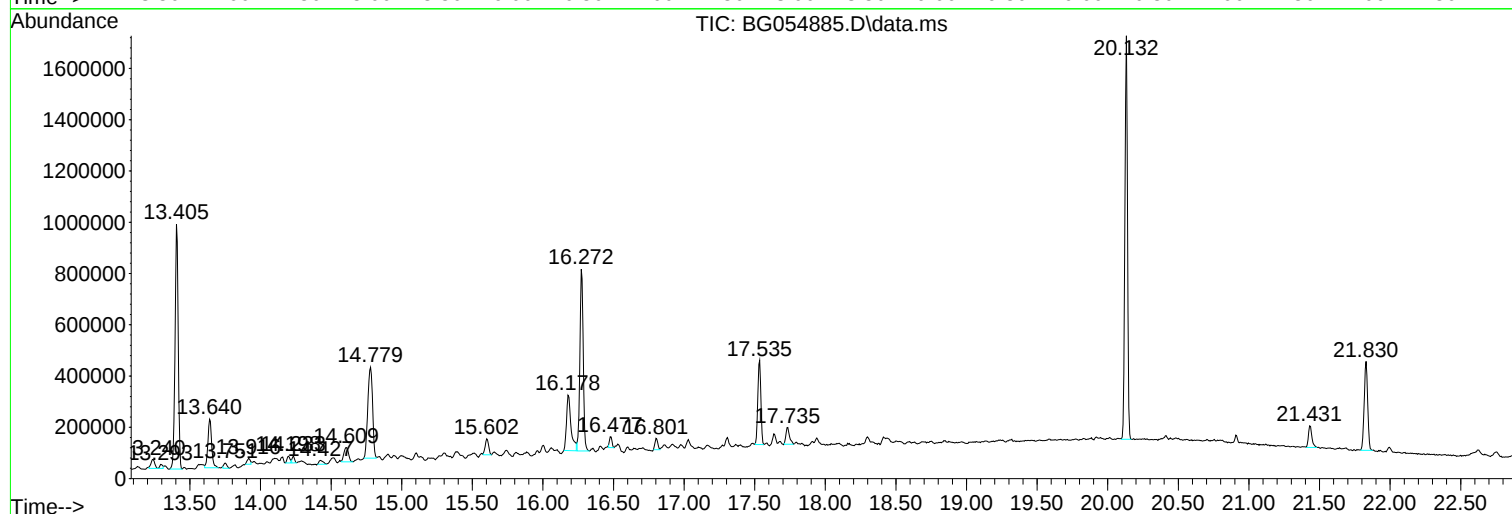
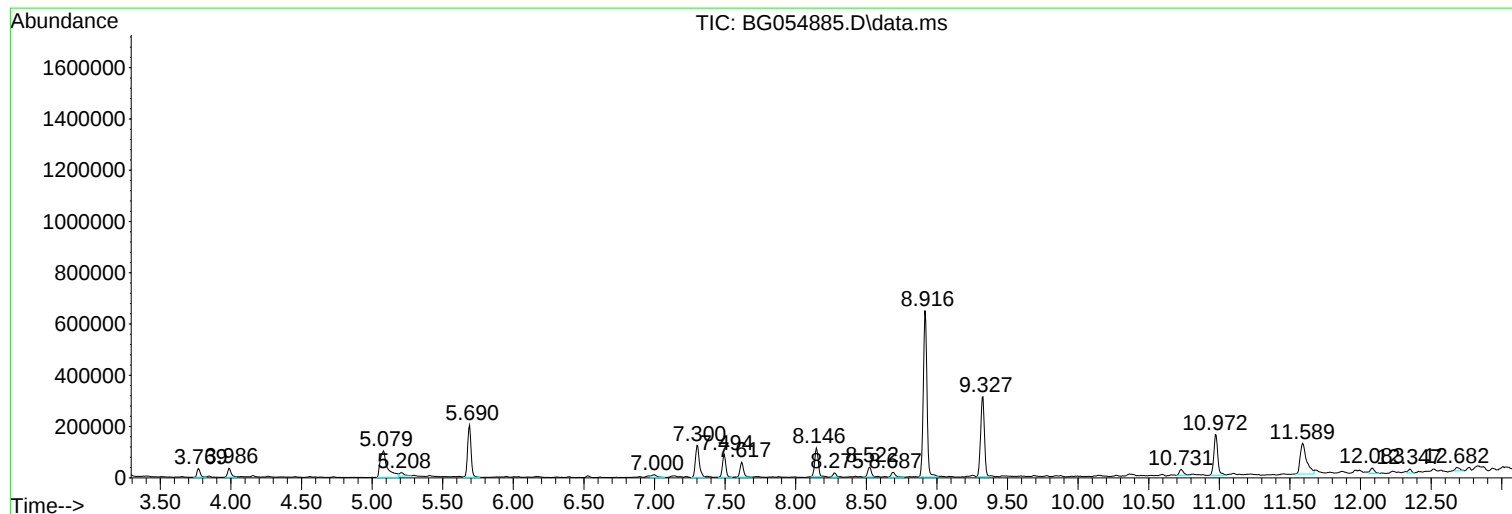
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW2

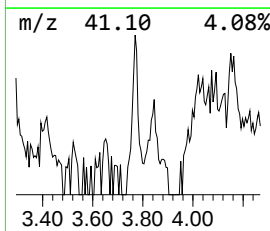
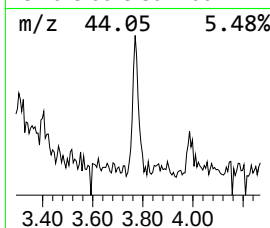
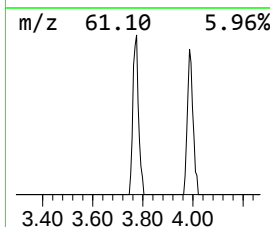
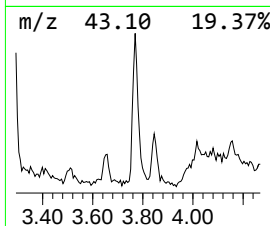
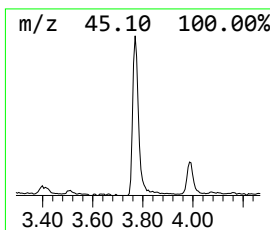
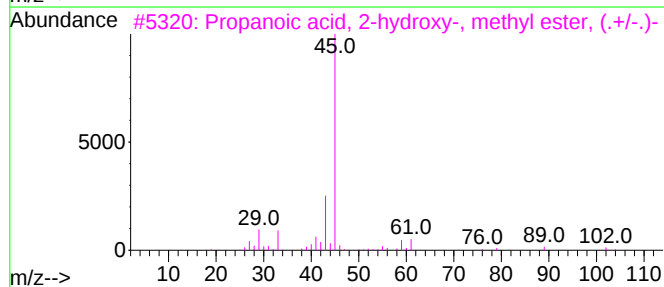
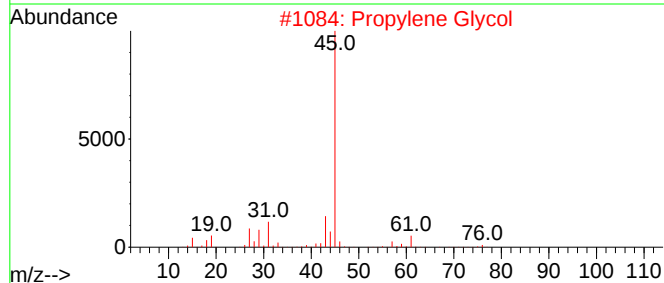
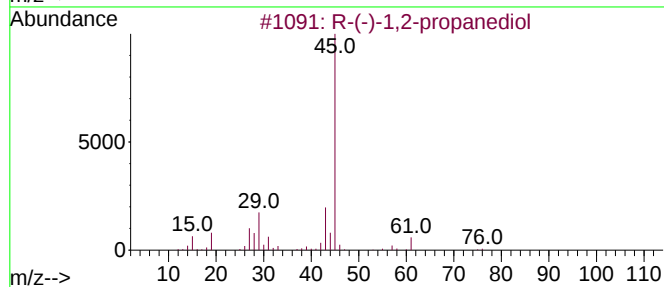
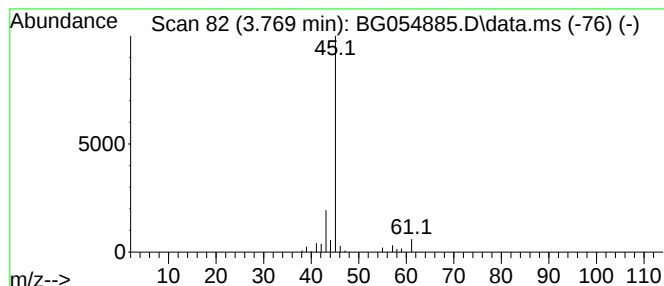
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.769 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.769	5.78 ng	55493	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	R(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
2	Propylene Glycol			76	C3H8O2	000057-55-6	43
3	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	40
4	Butane, 1-methoxy-			88	C5H12O	000628-28-4	9
5	Isopropyl Alcohol			60	C3H8O	000067-63-0	9



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Instrument :
BNA_G
ClientSampleId :
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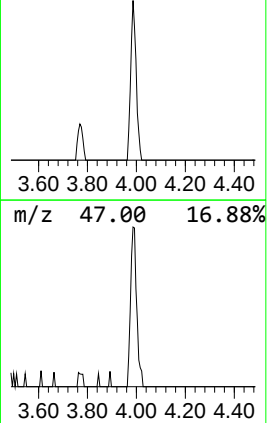
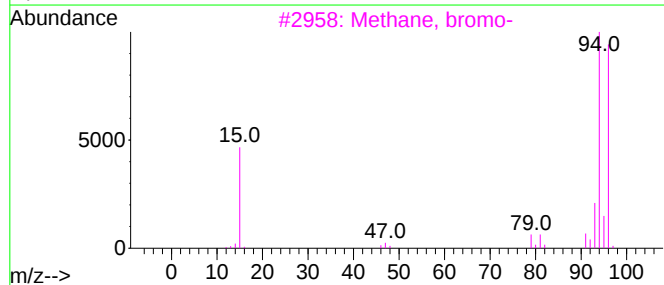
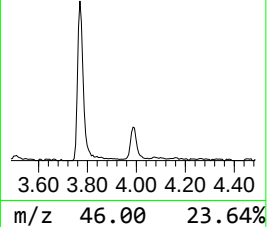
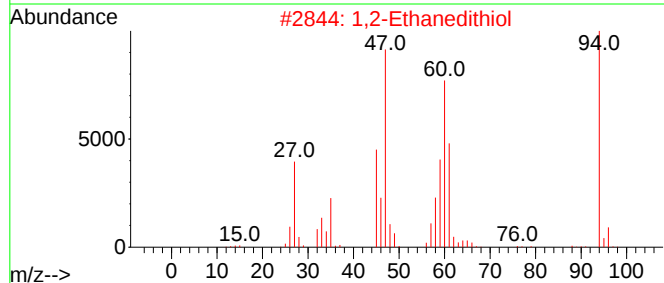
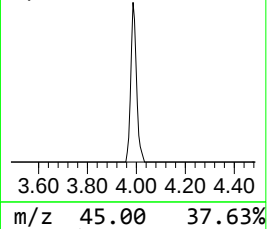
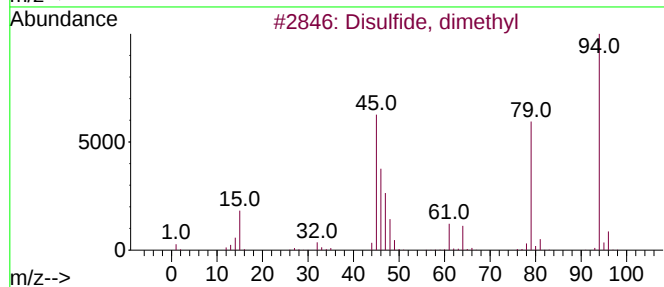
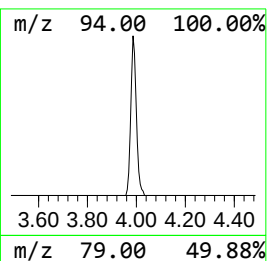
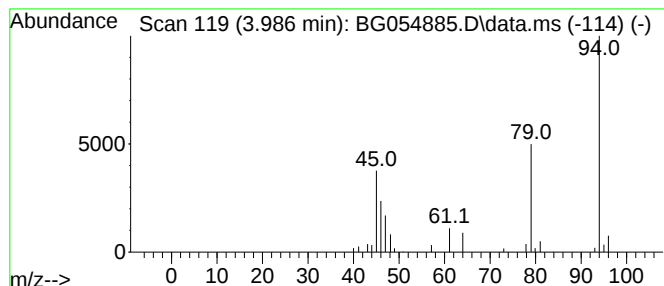
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Disulfide, dimethyl Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.986	6.50 ng	62397	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
2			1,2-Ethanedithiol	94	C2H6S2	000540-63-6	47
3			Methane, bromo-	94	CH3Br	000074-83-9	5
4			Ethanol	46	C2H6O	000064-17-5	4
5			4-Aminopyridine	94	C5H6N2	000504-24-5	4



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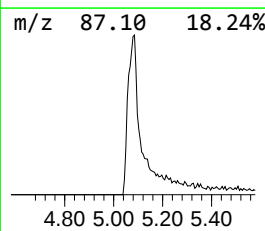
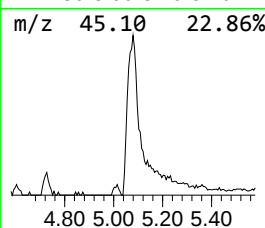
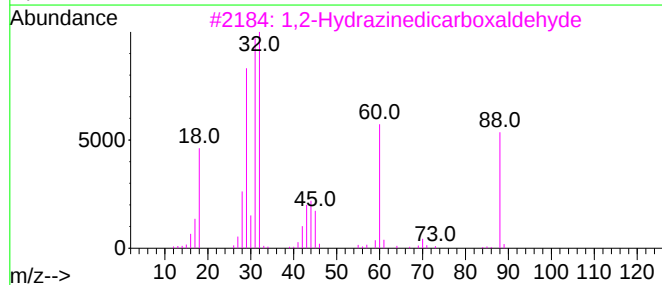
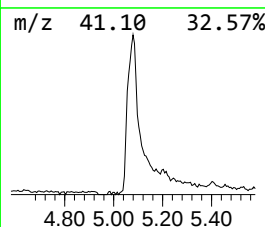
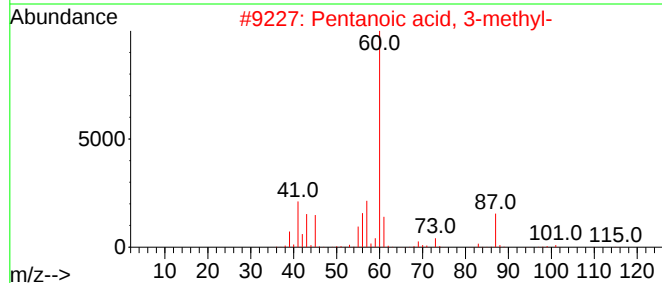
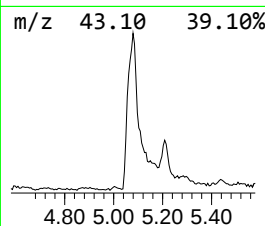
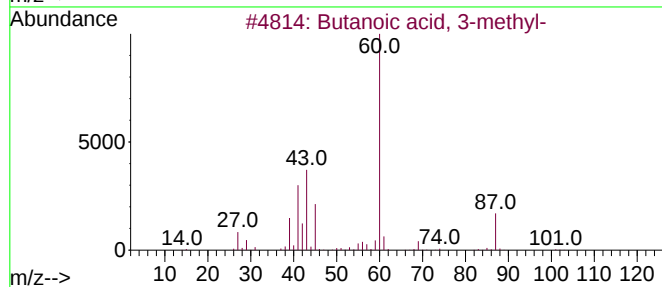
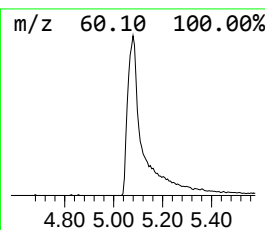
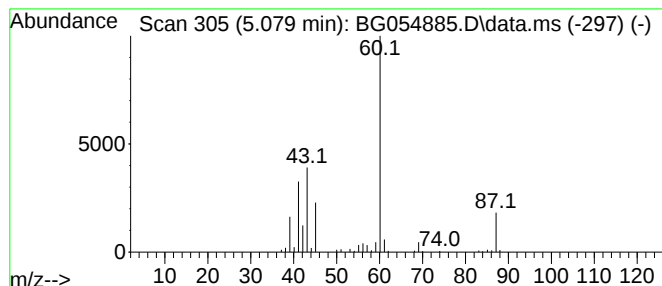
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.079	38.35 ng	367960	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	90
2			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	40
3			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	38
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5			1-Pentanamine	87	C5H13N	000110-58-7	9



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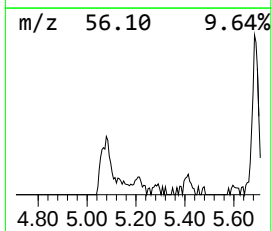
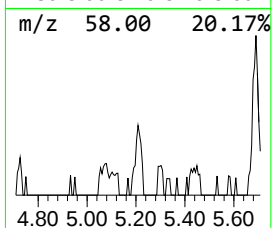
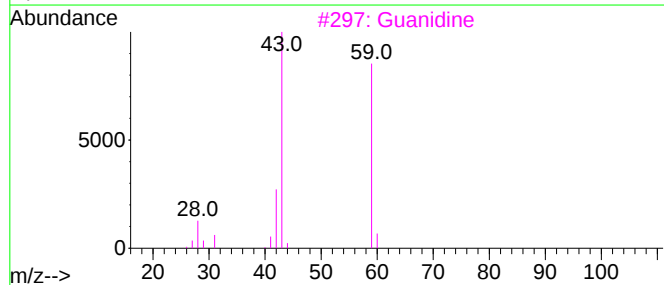
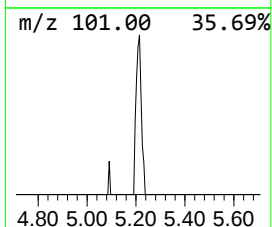
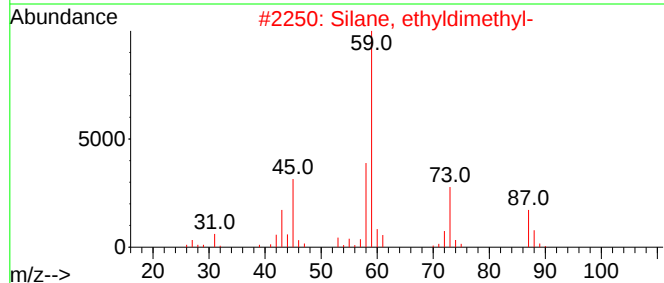
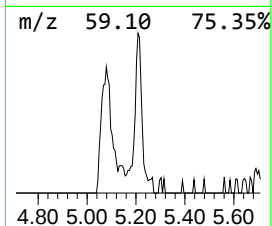
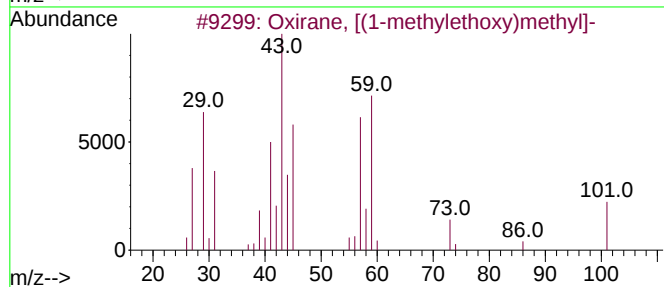
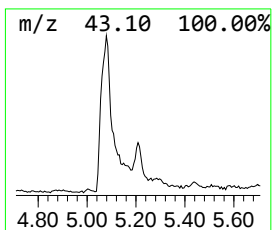
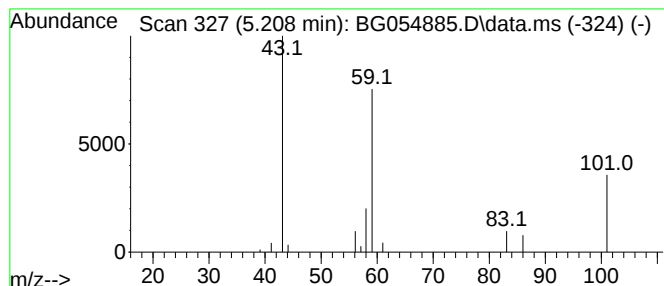
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown5.208 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.208	3.19 ng	30602	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	43
2			Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	28
3			Guanidine	59	CH5N3	000113-00-8	9
4			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	9
5			1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	9



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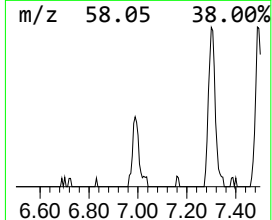
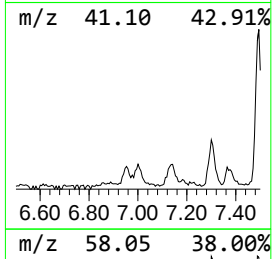
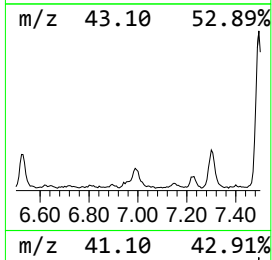
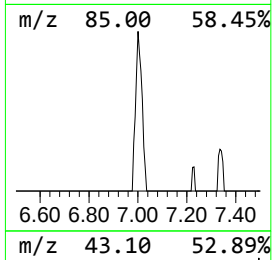
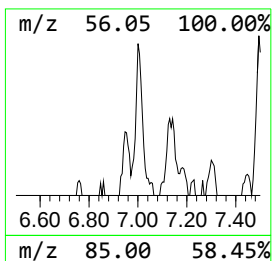
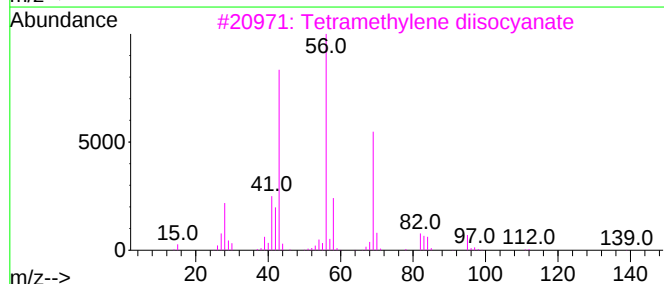
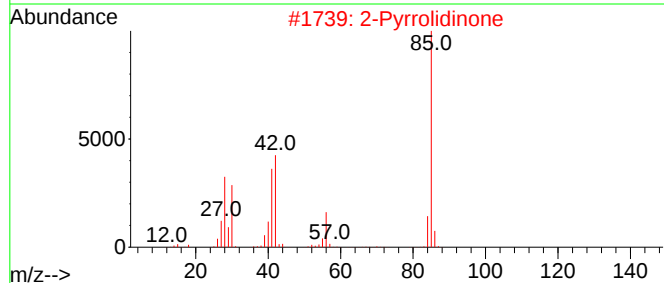
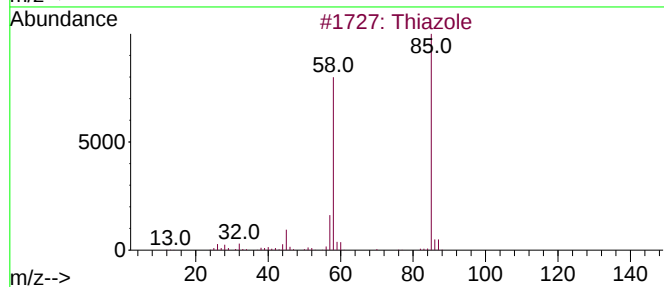
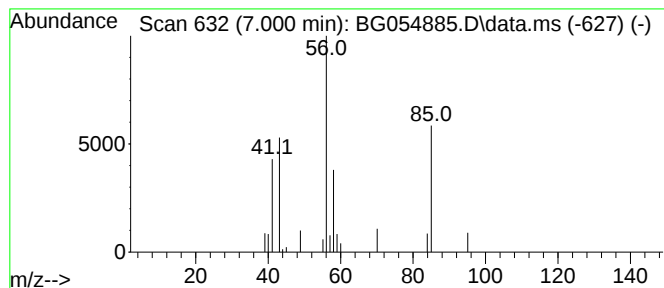
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown7.000 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.000	2.84 ng	27207	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiazole	85	C3H3NS	000288-47-1	9
2			2-Pyrrolidinone	85	C4H7NO	000616-45-5	9
3			Tetramethylene diisocyanate	140	C6H8N2O2	004538-37-8	9
4			1-Hexanol	102	C6H14O	000111-27-3	9
5			Cyclooctanamine	127	C8H17N	005452-37-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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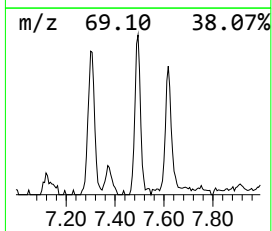
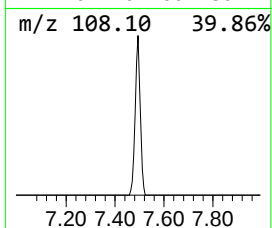
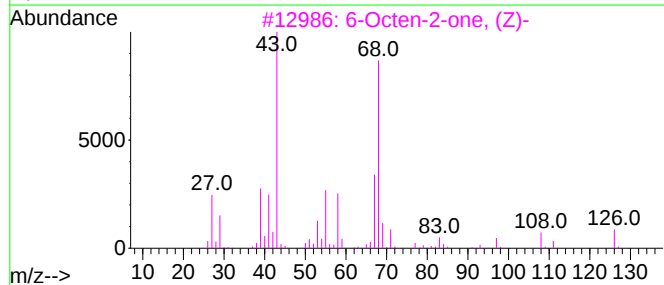
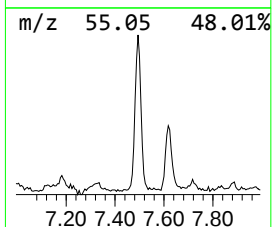
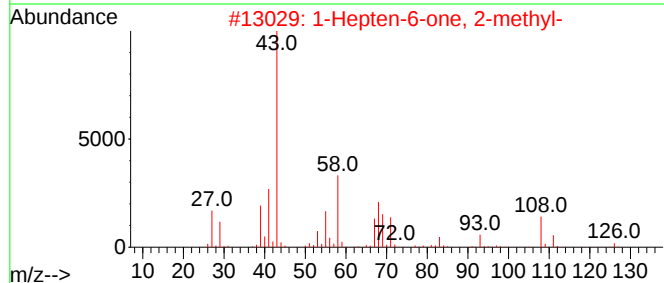
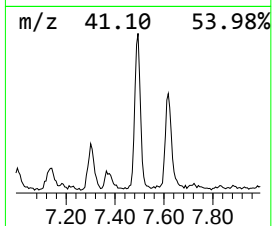
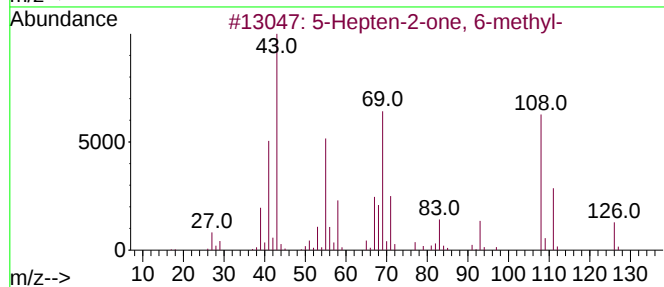
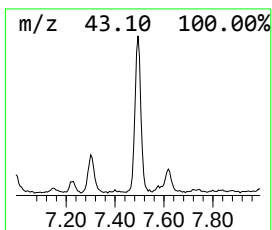
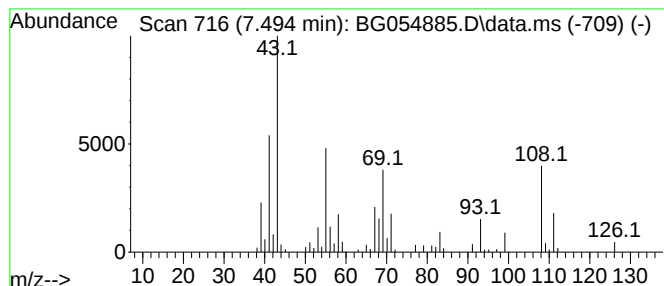
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Hepten-2-one, 6-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.494	15.43 ng	148029	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	86
2			1-Hepten-6-one, 2-methyl-	126	C8H14O	010408-15-8	47
3			6-Octen-2-one, (Z)-	126	C8H14O	074810-53-0	22
4			endo-2-Methyl-2-norbornanol	126	C8H14O	003212-16-6	16
5			7-Octen-2-one	126	C8H14O	003664-60-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
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Sample : N4537-02
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Instrument :
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ClientSampleId :
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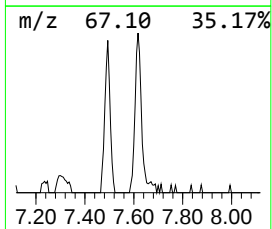
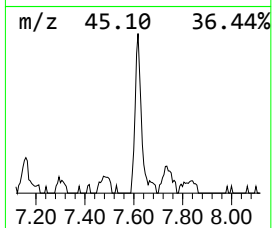
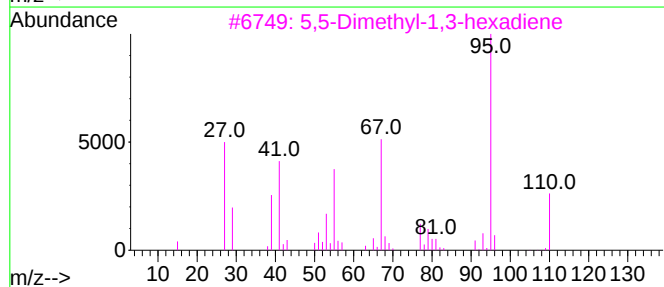
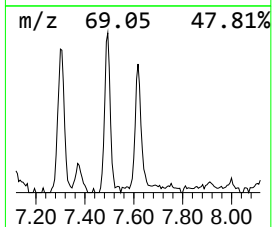
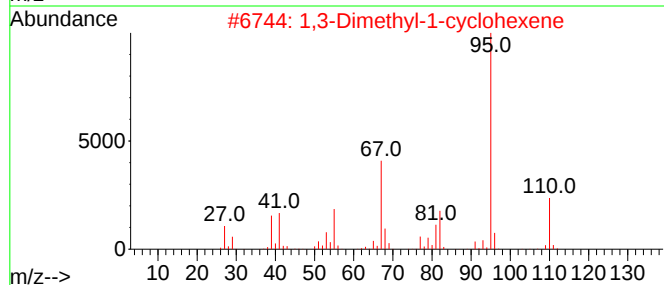
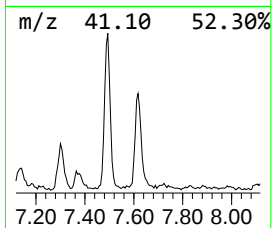
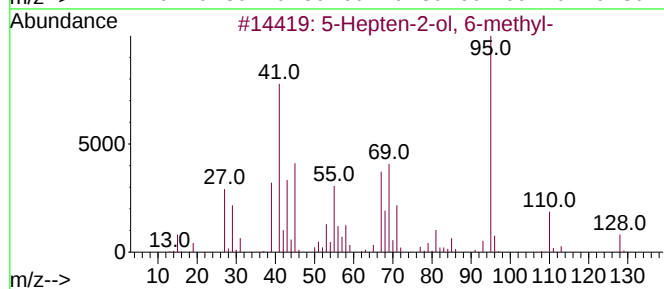
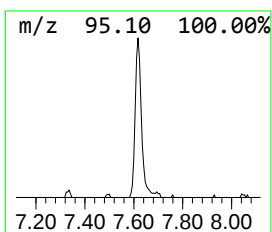
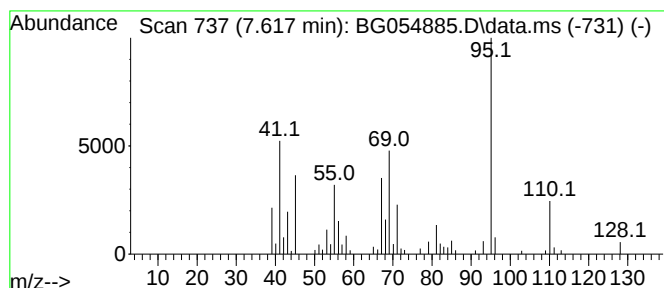
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Hepten-2-ol, 6-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.617	10.51 ng	100820	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Hepten-2-ol, 6-methyl-	128	C8H16O	001569-60-4	87
2			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	70
3			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	50
4			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	50
5			trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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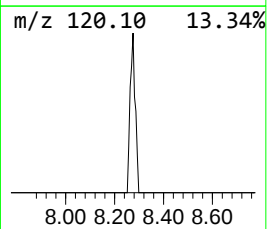
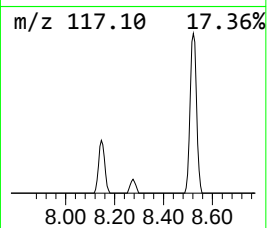
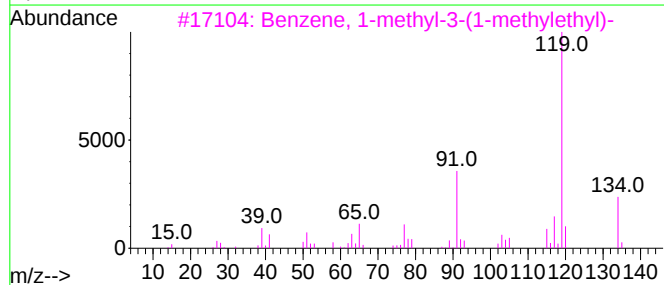
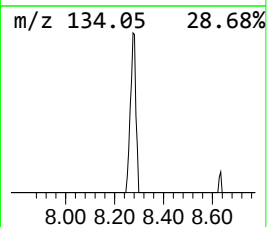
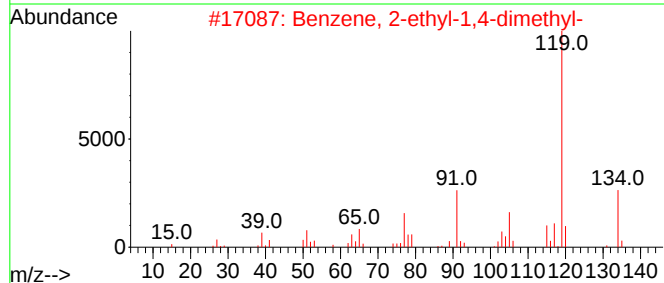
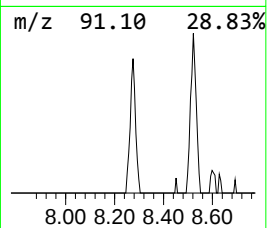
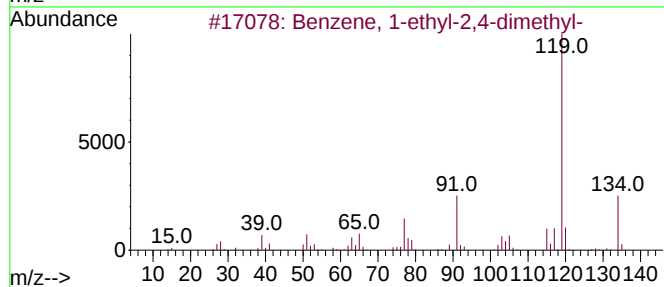
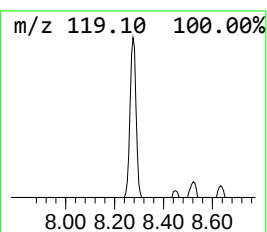
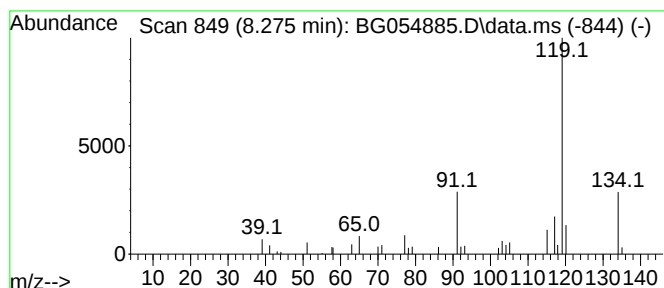
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.275	2.73 ng	26204	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91
4			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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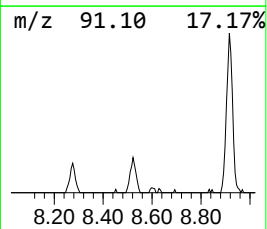
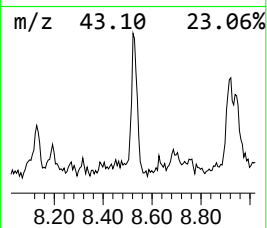
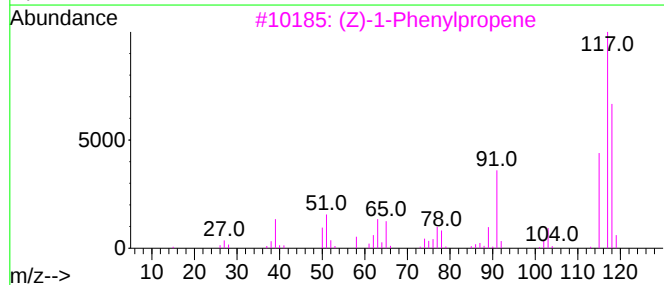
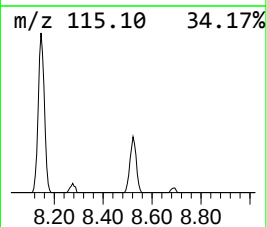
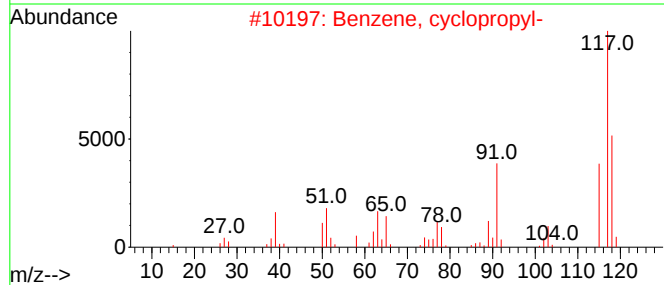
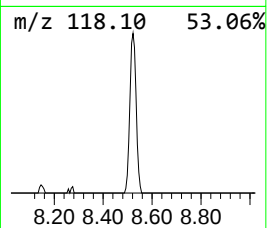
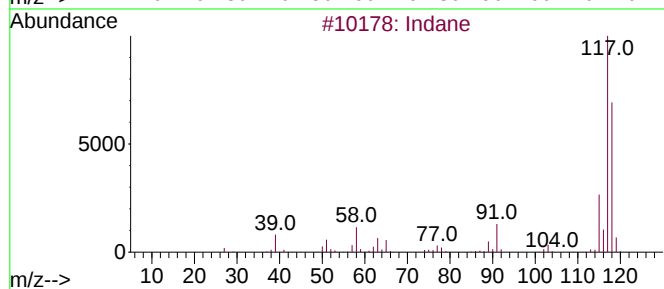
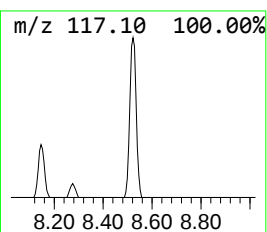
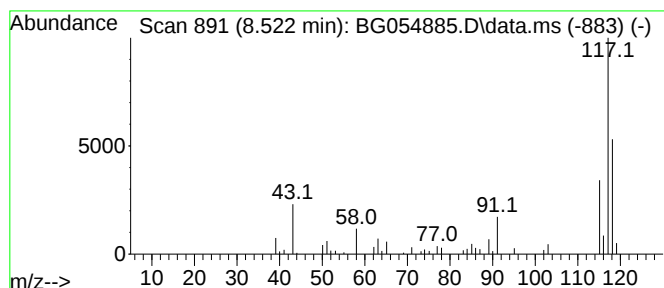
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.522	7.12 ng	68356	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	76
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
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Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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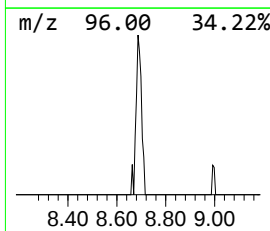
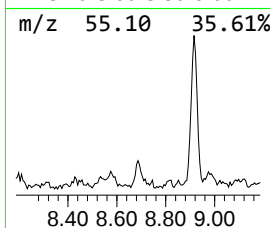
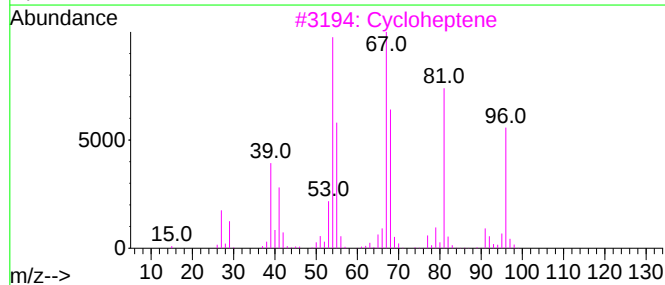
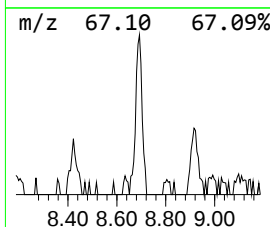
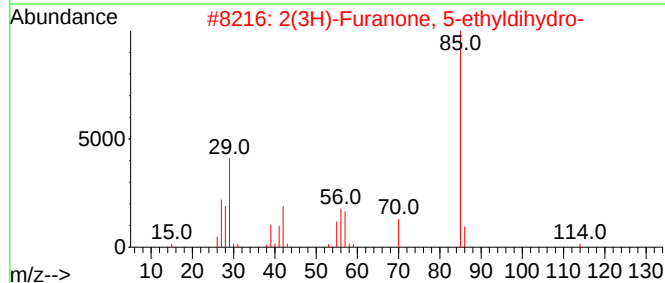
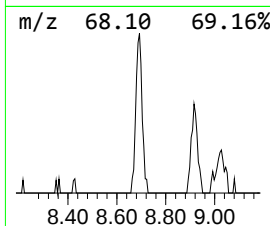
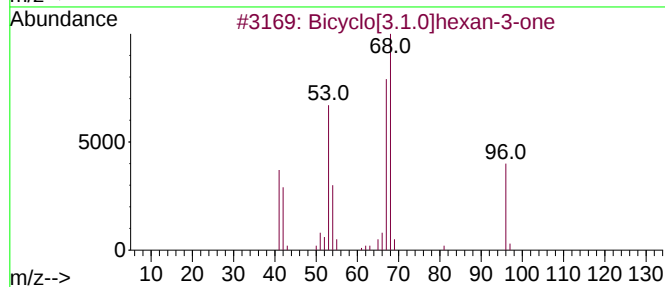
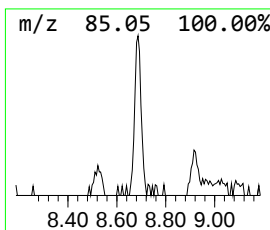
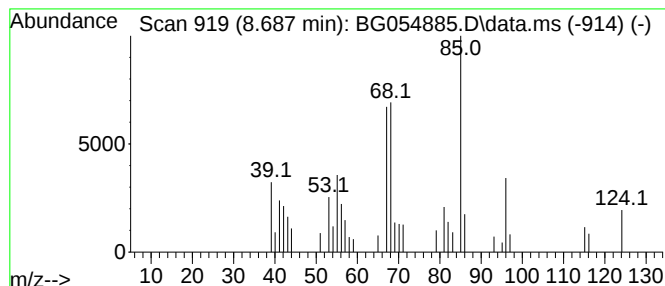
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown8.687 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.687	4.22 ng	40478	1,4-Dichlorobenzene-d4	8.146

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[3.1.0]hexan-3-one	96	C6H8O	001755-04-0	38
2		2(3H)-Furanone, 5-ethyldihydro-	114	C6H10O2	000695-06-7	35
3		Cycloheptene	96	C7H12	000628-92-2	27
4		Tetrahydropyran 12-tetradecyn-1-...	294	C19H34O2	096249-40-0	27
5		Oxirane, 2-methyl-2-pentyl-	128	C8H16O	053907-75-8	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
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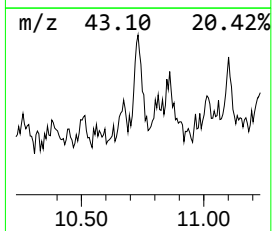
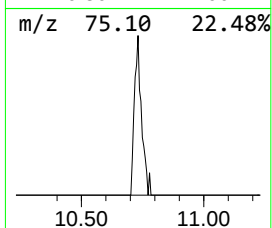
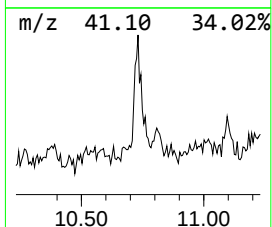
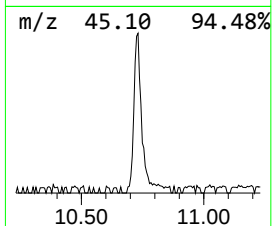
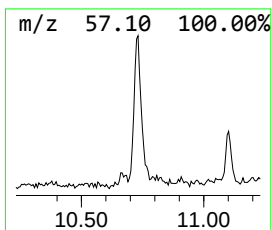
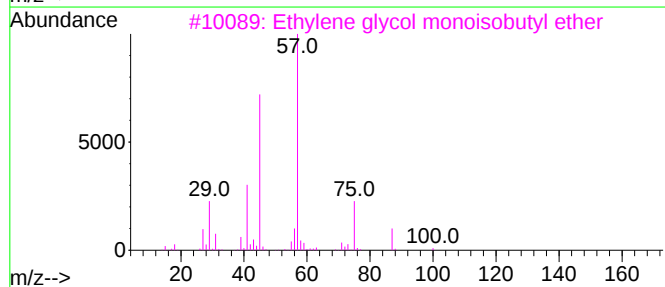
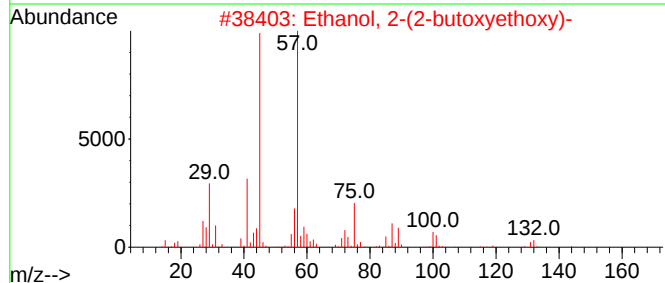
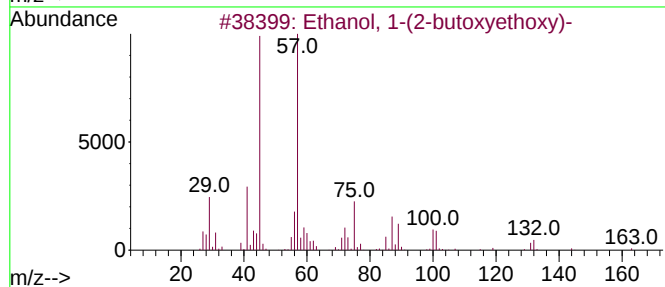
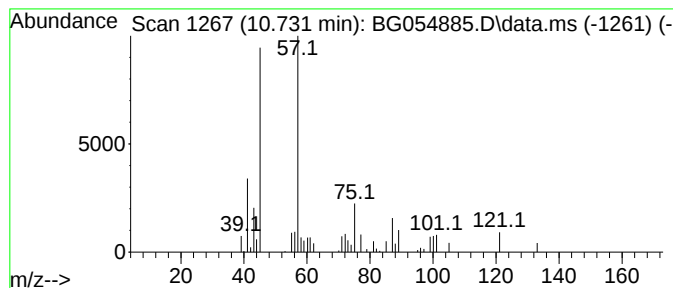
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.731	3.10 ng	47688	Naphthalene-d8	10.972	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	72
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	43
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

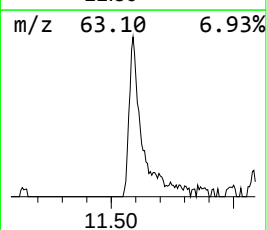
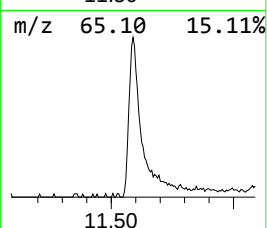
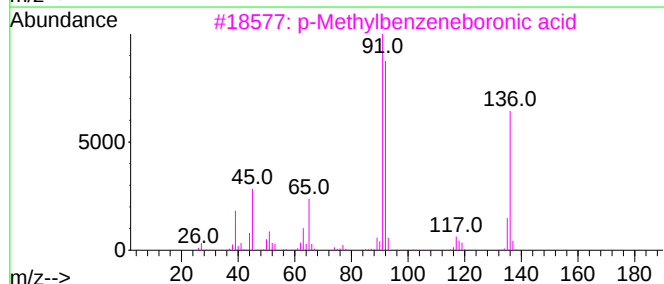
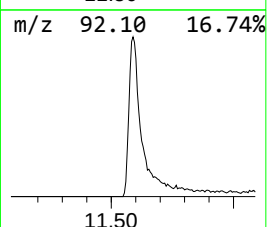
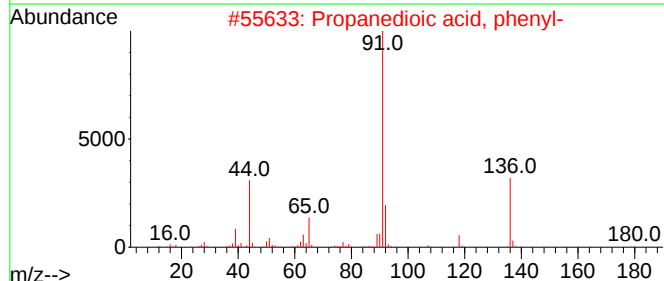
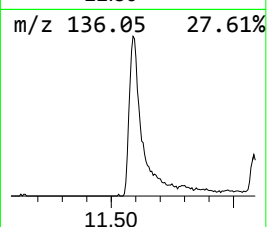
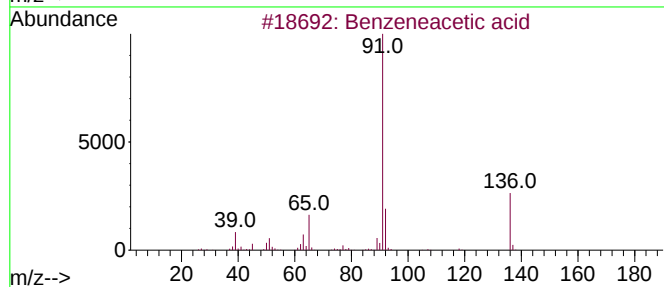
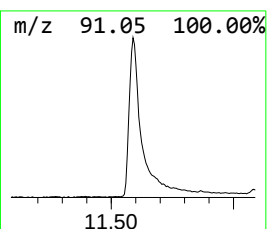
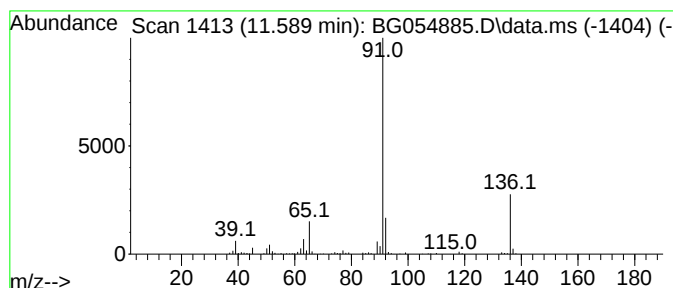
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzeneacetic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.589	24.75 ng	380552	Naphthalene-d8	10.972	
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	72
3	p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	59
4	Phenylacetic acid, pent-2-en-4-y...	200	C13H12O2	1000292-61-1	53
5	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

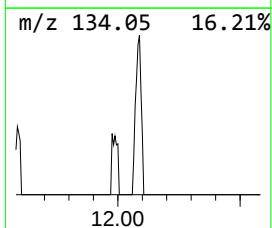
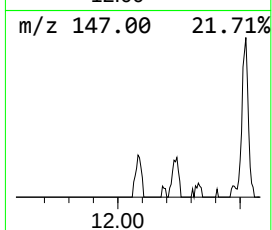
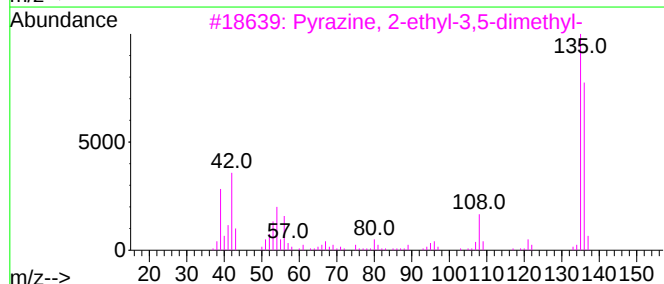
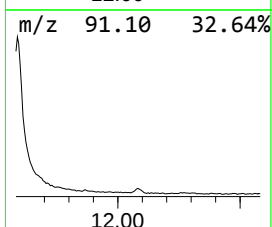
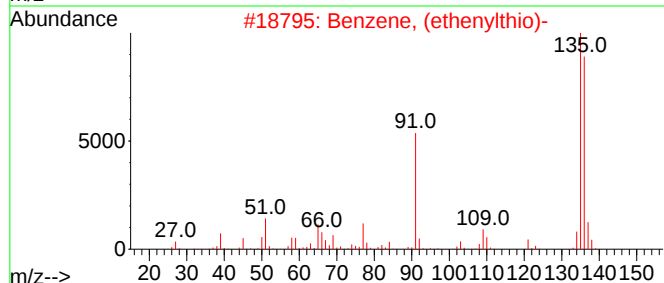
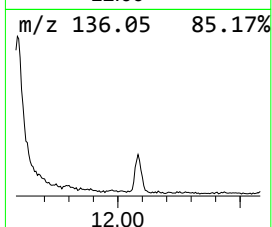
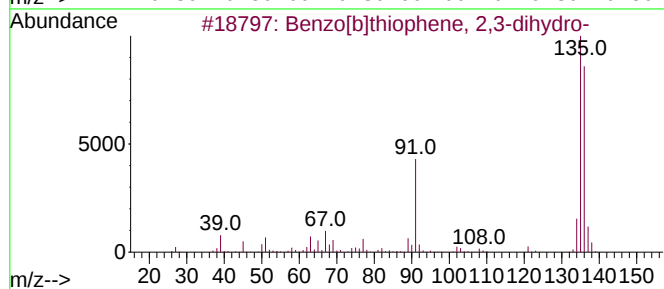
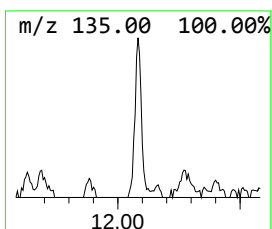
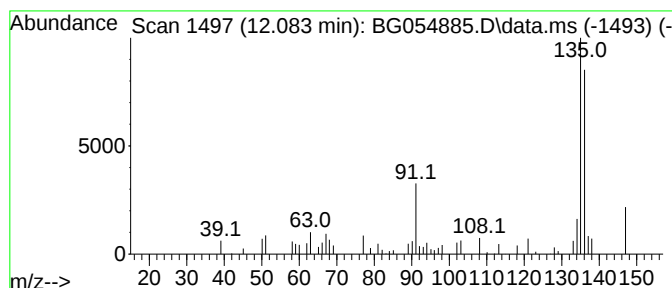
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzo[b]thiophene, 2,3-dihy... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.083	2.70 ng	41554	Naphthalene-d8	10.972	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]thiophene, 2,3-dihydro-	136	C8H8S	004565-32-6	74
2	Benzene, (ethenylthio)-	136	C8H8S	001822-73-7	72
3	Pyrazine, 2-ethyl-3,5-dimethyl-	136	C8H12N2	013925-07-0	64
4	Benzaldehyde, 4-methoxy-	136	C8H8O2	000123-11-5	64
5	2-Hydroxy-5-methylbenzaldehyde	136	C8H8O2	000613-84-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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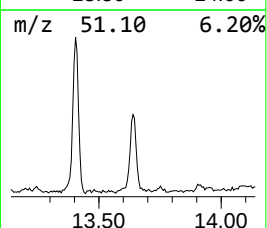
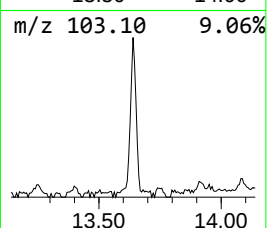
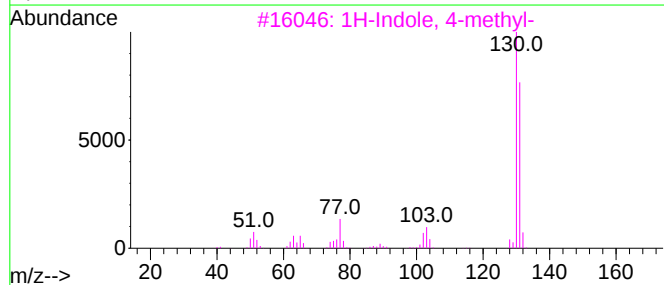
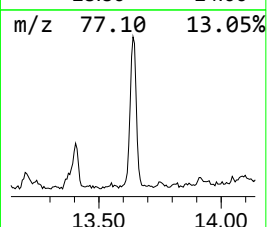
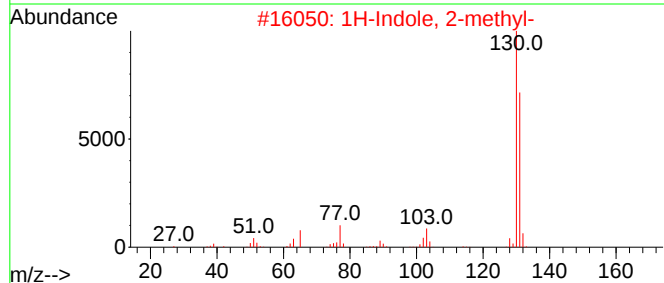
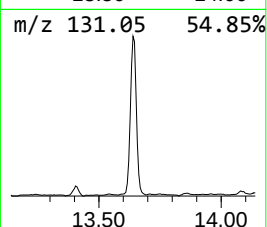
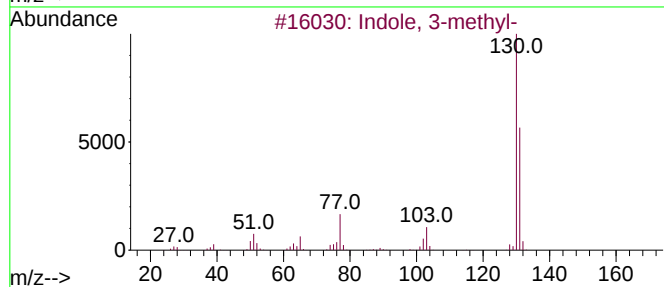
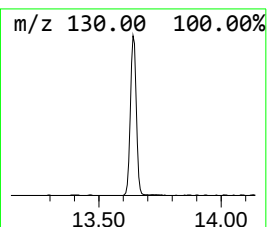
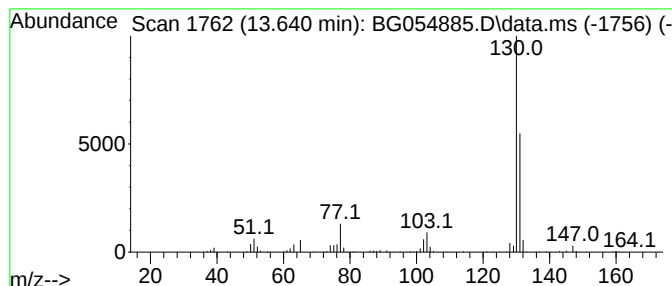
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Indole, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.640	8.35 ng	348510	Acenaphthene-d10	14.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Indole, 3-methyl-	131	C9H9N	000083-34-1	95
2		1H-Indole, 2-methyl-	131	C9H9N	000095-20-5	91
3		1H-Indole, 4-methyl-	131	C9H9N	016096-32-5	91
4		1H-Indole, 5-methyl-	131	C9H9N	000614-96-0	91
5		Indolizine, 3-methyl-	131	C9H9N	001761-10-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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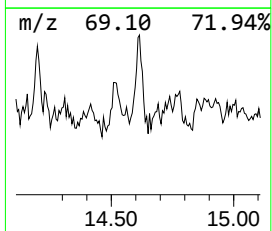
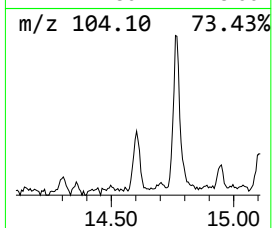
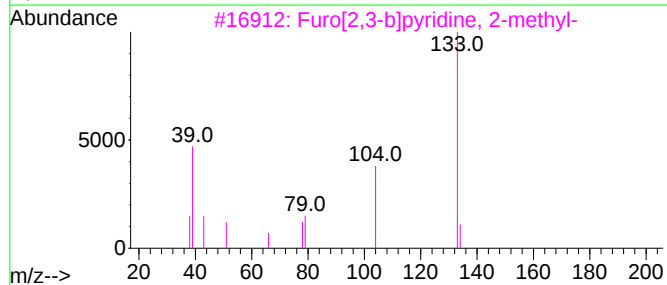
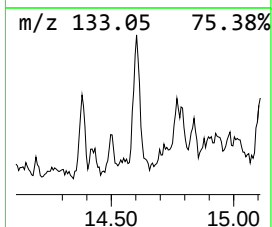
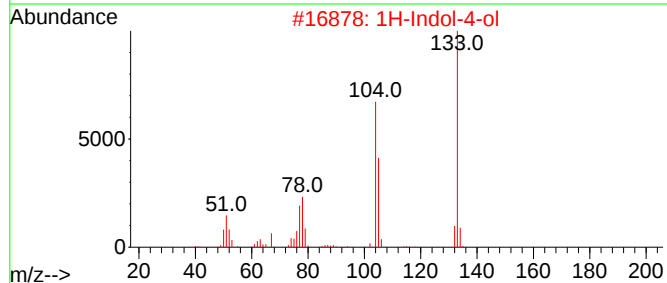
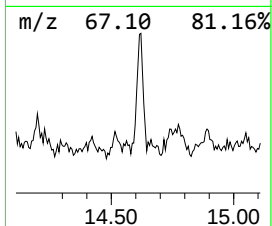
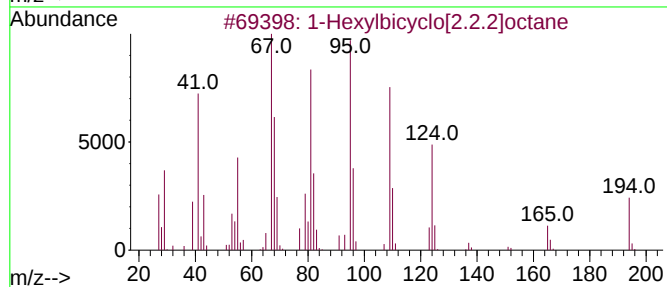
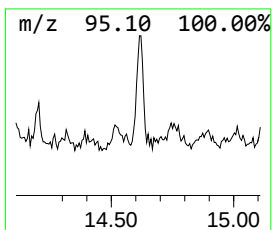
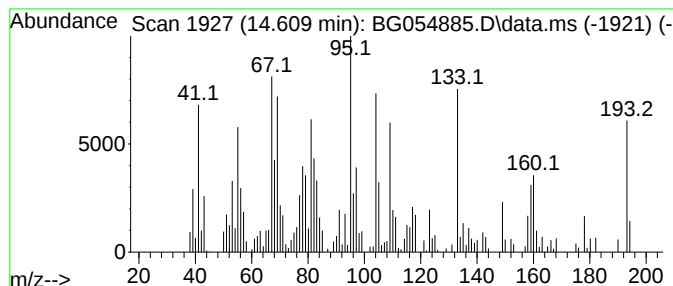
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1-Hexylbicyclo[2.2.2]octane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.609	3.06 ng	127586	Acenaphthene-d10	14.785

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexylbicyclo[2.2.2]octane	194	C14H26	1000435-94-2	52
2			1H-Indol-4-ol	133	C8H7NO	002380-94-1	38
3			Furo[2,3-b]pyridine, 2-methyl-	133	C8H7NO	075332-26-2	35
4			Benzene, 1-isocyanato-2-methyl-	133	C8H7NO	000614-68-6	35
5			3-(4-Pyridyl)acrylaldehyde	133	C8H7NO	026505-36-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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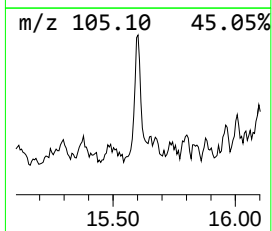
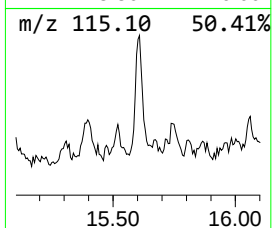
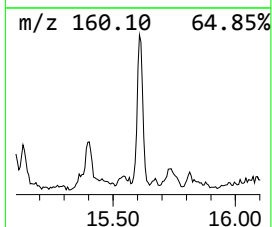
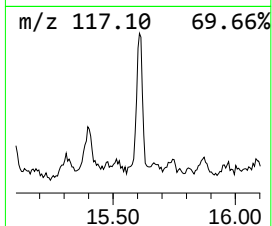
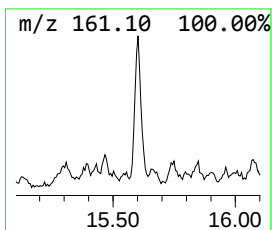
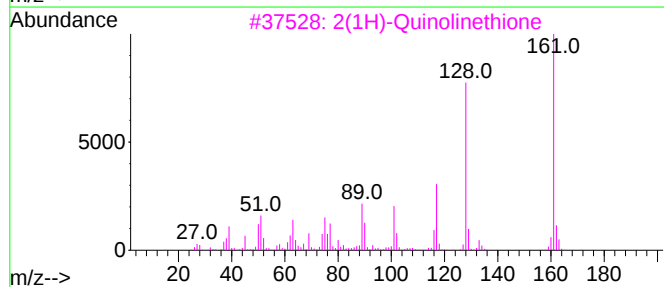
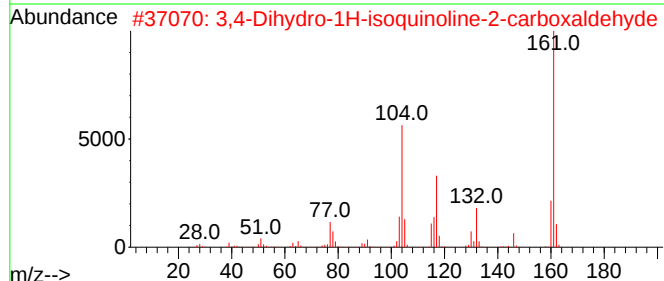
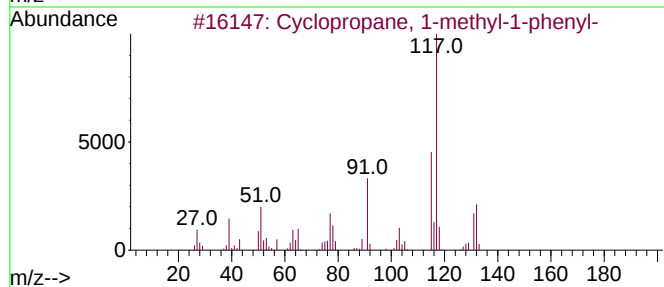
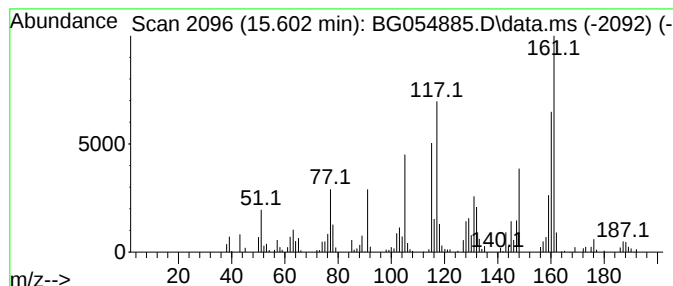
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown15.602 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.602	2.47 ng	102977	Acenaphthene-d10	14.785

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	41
2		3,4-Dihydro-1H-isoquinoline-2-ca...	161	C10H11NO	001699-52-1	38
3		2(1H)-Quinolinethione	161	C9H7NS	002637-37-8	25
4		3-Hydroxymethylene-2-indolinone	161	C9H7NO2	063273-23-4	25
5		1H-Inden-1-one, 2,3-dihydro-4,7-...	160	C11H12O	005037-60-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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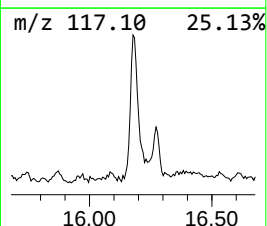
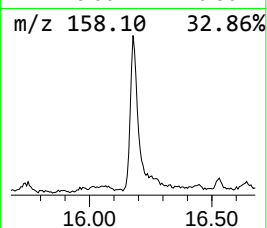
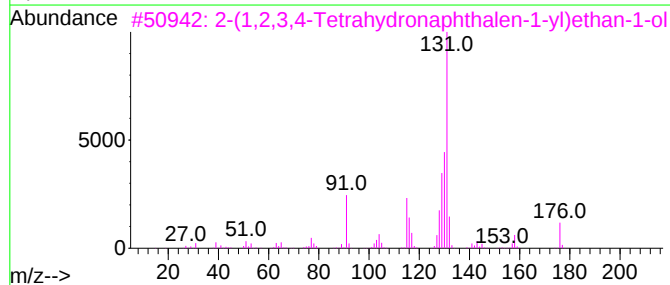
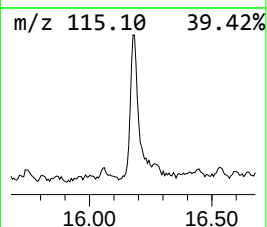
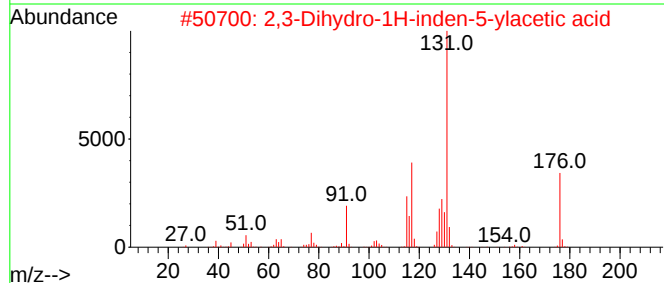
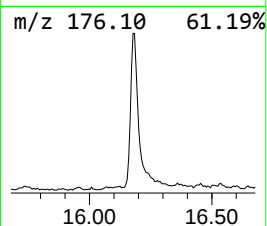
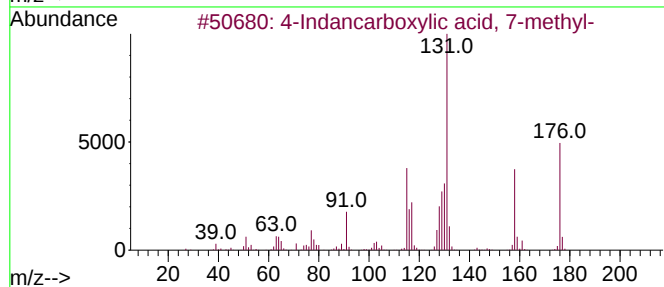
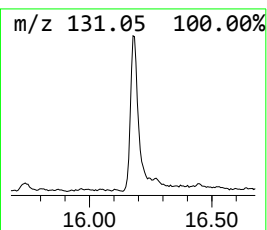
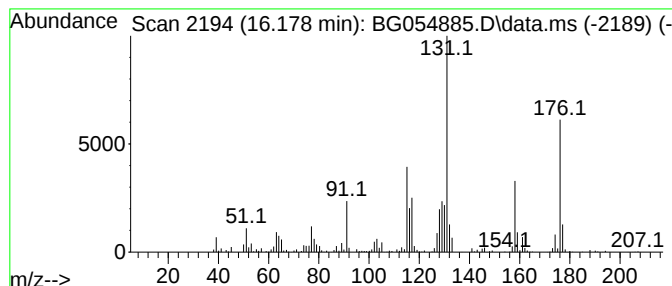
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 4-Indancarboxylic acid, 7-m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.178	19.49 ng	475676	Phenanthrene-d10	17.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Indancarboxylic acid, 7-methyl-	176	C11H12O2	071042-74-5	97
2			2,3-Dihydro-1H-inden-5-ylacetic ...	176	C11H12O2	005453-98-5	90
3			2-(1,2,3,4-Tetrahydronaphthalen-...	176	C12H16O	068480-12-6	76
4			1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	72
5			1-(p-Tolyl)cyclopropanecarboxyli...	176	C11H12O2	083846-66-6	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
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Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

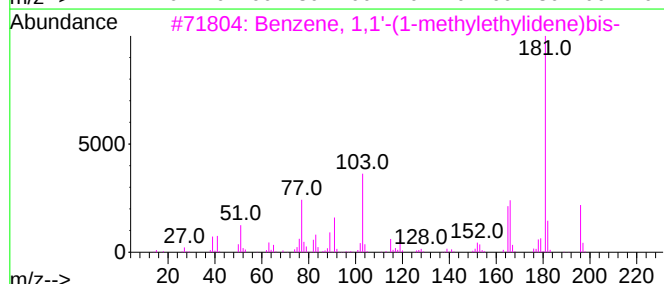
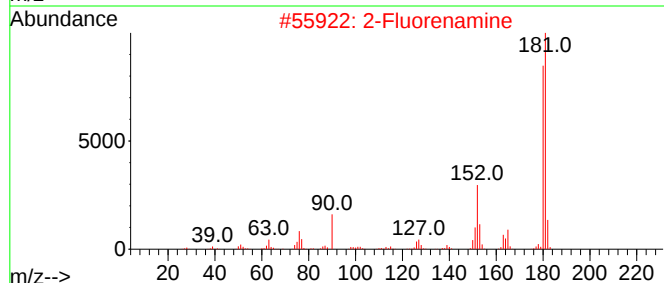
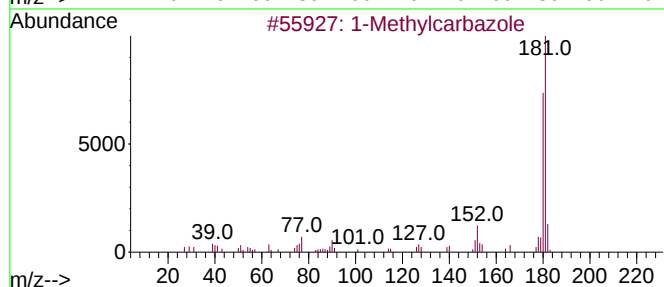
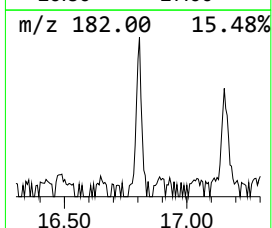
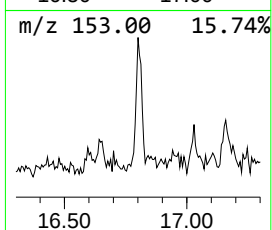
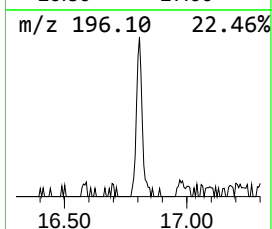
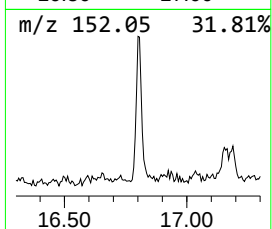
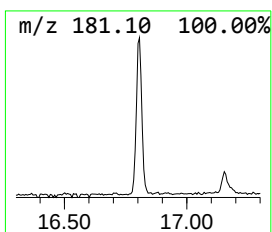
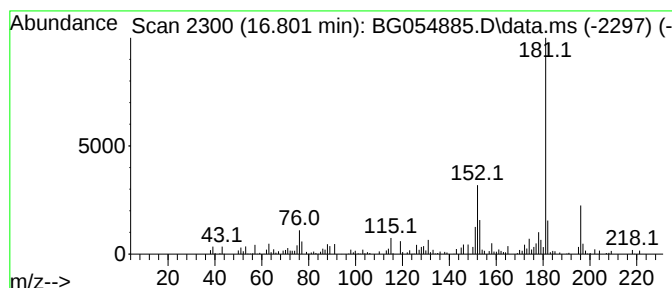
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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 1-Methylcarbazole Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.801	2.58 ng	62844	Phenanthrene-d10	17.535	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylcarbazole	181	C13H11N	006510-65-2	80
2	2-Fluorenamine	181	C13H11N	000153-78-6	72
3	Benzene, 1,1'-(1-methylethyliden...	196	C15H16	000778-22-3	64
4	(1,1'-Biphenyl)-2,2'-dicarboxald...	210	C14H10O2	001210-05-5	59
5	4-Methylcarbazole	181	C13H11N	003770-48-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW2

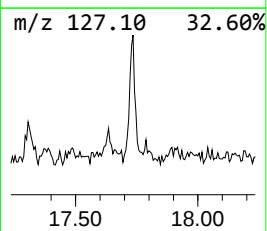
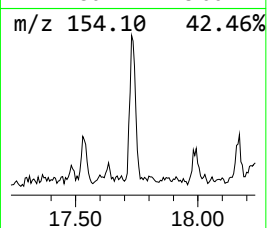
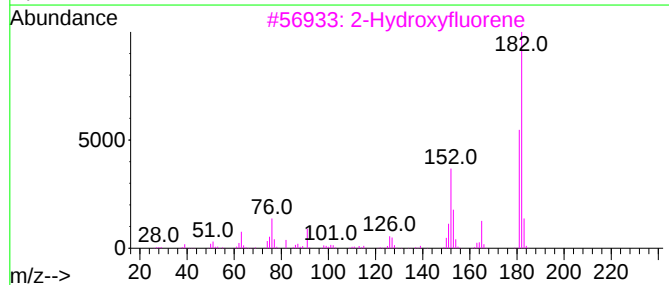
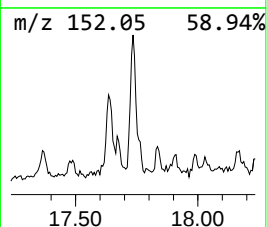
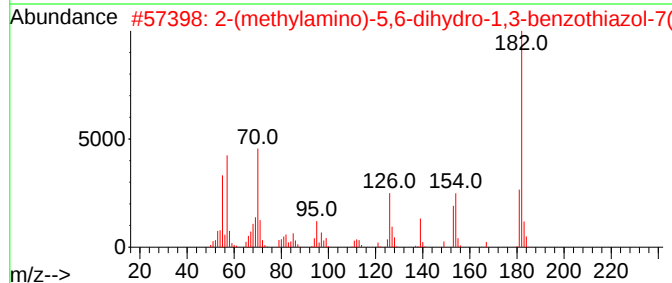
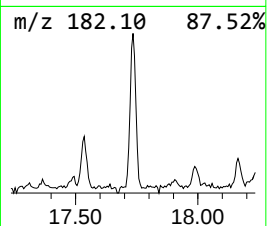
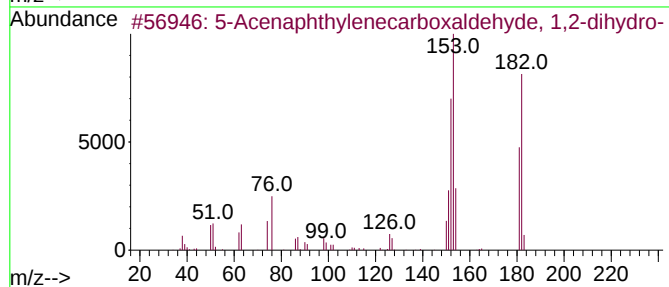
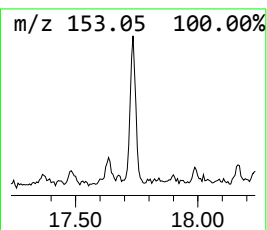
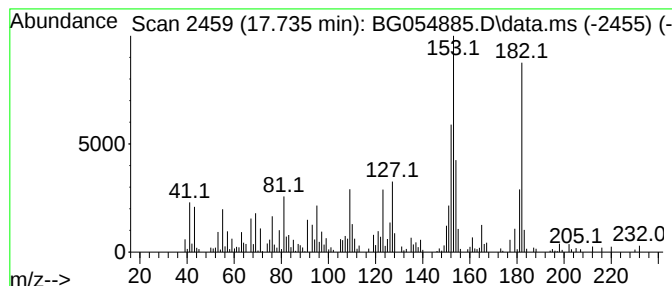
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 5-Acenaphthylenecarboxalde... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.735	4.72 ng	115257	Phenanthrene-d10	17.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Acenaphthylenecarboxaldehyde, ...	182	C13H10O	1000362-64-3	58
2			2-(methylamino)-5,6-dihydro-1,3-...	182	C8H10N2OS	1000285-58-7	43
3			2-Hydroxyfluorene	182	C13H10O	002443-58-5	38
4			3,5-Dimethoxybenzoic acid	182	C9H10O4	001132-21-4	35
5			2-(2-Aminoethyl)-4-amino-6-dimet...	182	C7H14N6	040917-13-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

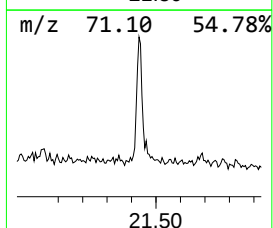
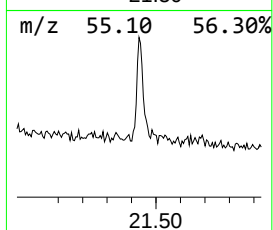
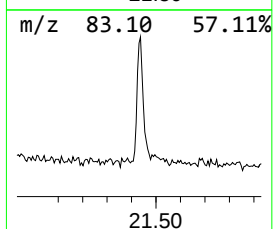
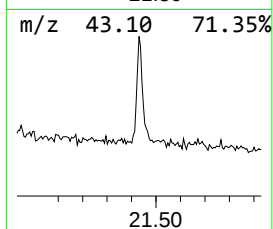
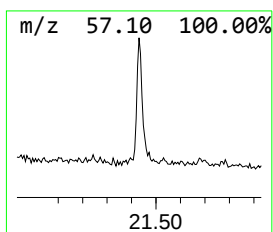
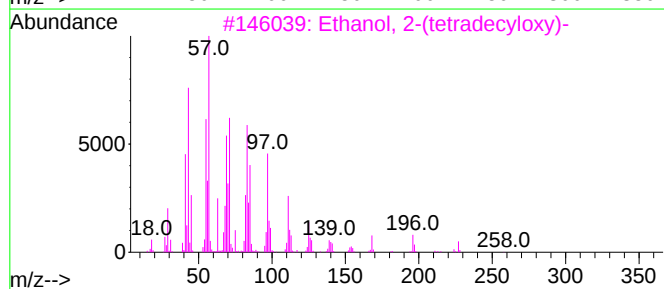
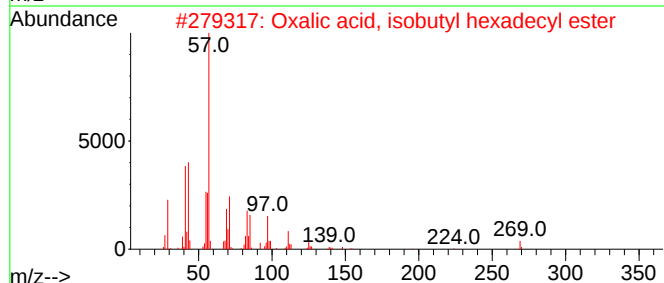
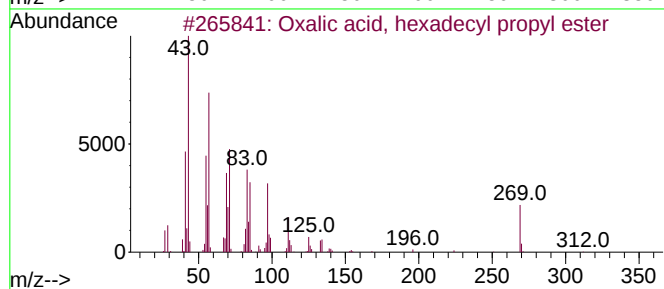
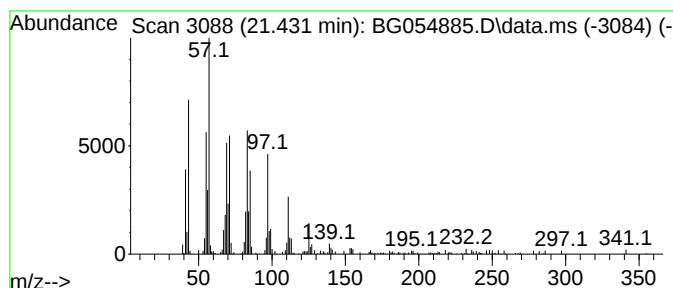
Instrument :
BNA_G
ClientSampleId :
MW2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Oxalic acid, hexadecyl prop... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.430	4.85 ng	142594	Chrysene-d12		21.830	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Oxalic acid, hexadecyl propyl ester		356	C21H40O4	1000309-26-9	91
2	Oxalic acid, isobutyl hexadecyl ...		370	C22H42O4	1000309-38-1	91
3	Ethanol, 2-(tetradecyloxy)-		258	C16H34O2	002136-70-1	91
4	Docosyl pentafluoropropionate		472	C25H45F5O2	1000351-80-9	91
5	1-Hexadecanesulfonyl chloride		324	C16H33ClO2S	038775-38-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054885.D
Acq On : 8 Sep 2022 15:45
Operator : CG/JU
Sample : N4537-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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
unknown3.769	3.769	5.8	ng	55493	1	8.146	191900	20.0
Disulfide, dime...	3.986	6.5	ng	62397	1	8.146	191900	20.0
Butanoic acid, ...	5.079	38.4	ng	367960	1	8.146	191900	20.0
unknown5.208	5.208	3.2	ng	30602	1	8.146	191900	20.0
unknown7.000	7.000	2.8	ng	27207	1	8.146	191900	20.0
5-Hepten-2-one,...	7.494	15.4	ng	148029	1	8.146	191900	20.0
5-Hepten-2-ol, ...	7.617	10.5	ng	100820	1	8.146	191900	20.0
Benzene, 1-ethy...	8.275	2.7	ng	26204	1	8.146	191900	20.0
Indane	8.522	7.1	ng	68356	1	8.146	191900	20.0
unknown8.687	8.687	4.2	ng	40478	1	8.146	191900	20.0
Ethanol, 1-(2-b...	10.731	3.1	ng	47688	2	10.972	307513	20.0
Benzeneacetic acid	11.589	24.8	ng	380552	2	10.972	307513	20.0
Benzo[b]thiophe...	12.083	2.7	ng	41554	2	10.972	307513	20.0
Indole, 3-methyl-	13.640	8.3	ng	348510	3	14.785	834612	20.0
1-Hexylbicyclo[...	14.609	3.1	ng	127586	3	14.785	834612	20.0
unknown15.602	15.602	2.5	ng	102977	3	14.785	834612	20.0
4-Indancarboxyl...	16.178	19.5	ng	475676	4	17.535	488049	20.0
1-Methylcarbazole	16.801	2.6	ng	62844	4	17.535	488049	20.0
5-Acenaphthylen...	17.735	4.7	ng	115257	4	17.535	488049	20.0
Oxalic acid, he...	21.430	4.8	ng	142594	5	21.830	588160	20.0