

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022822\
 Data File : BG052507.D
 Acq On : 28 Feb 2022 18:44
 Operator : CG/JU
 Sample : N1668-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PURGED-WATER

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-BG020722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052507.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.128	103	109	118	rVB2	20380	34671	1.09%	0.287%
2	5.262	297	302	308	rVB	20692	32094	1.01%	0.266%
3	5.750	378	385	395	rBV	295108	478882	15.08%	3.968%
4	6.255	461	471	484	rBV	321726	503093	15.84%	4.169%
5	7.365	653	660	671	rBV	201169	362875	11.42%	3.007%
6	8.217	800	805	809	rBV	95513	157228	4.95%	1.303%
7	8.264	809	813	823	rVB4	31648	73855	2.33%	0.612%
8	8.358	823	829	840	rVB5	24816	58900	1.85%	0.488%
9	8.910	917	923	932	rVB5	31231	55030	1.73%	0.456%
10	9.392	998	1005	1013	rVB	381645	676453	21.30%	5.605%
11	11.054	1281	1288	1298	rBV	136875	238759	7.52%	1.978%
12	12.335	1499	1506	1513	rBV	76673	126584	3.99%	1.049%
13	13.486	1694	1702	1709	rBV	1047116	1631887	51.37%	13.521%
14	13.698	1728	1738	1742	rBV	28977	51738	1.63%	0.429%
15	14.127	1804	1811	1818	rBV	35048	59348	1.87%	0.492%
16	14.861	1929	1936	1946	rVB	234431	380761	11.99%	3.155%
17	16.206	2159	2165	2174	rBV7	19324	47881	1.51%	0.397%
18	16.353	2183	2190	2203	rBV	881731	1396857	43.98%	11.574%
19	17.610	2399	2404	2410	rBV	324328	504989	15.90%	4.184%
20	18.997	2634	2640	2646	rBV2	22178	39578	1.25%	0.328%
21	19.872	2785	2789	2792	rBV	43949	57920	1.82%	0.480%
22	19.907	2792	2795	2799	rVB4	28470	35104	1.11%	0.291%
23	20.207	2837	2846	2855	rVB2	1903515	3176454	100.00%	26.319%
24	21.211	3011	3017	3023	rVB	487825	668876	21.06%	5.542%
25	21.617	3080	3086	3090	rBV	25848	44809	1.41%	0.371%
26	21.928	3132	3139	3147	rVB2	335688	559358	17.61%	4.635%
27	22.463	3224	3230	3237	rBV3	23251	40060	1.26%	0.332%
28	25.394	3718	3729	3740	rVB3	191534	574865	18.10%	4.763%

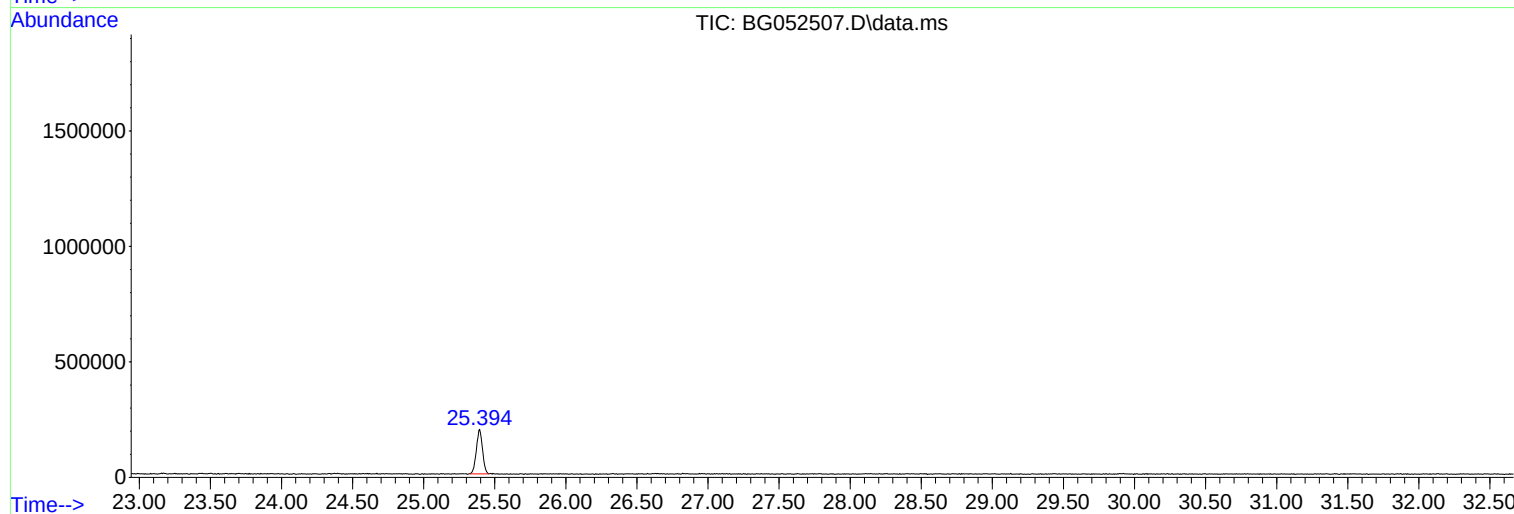
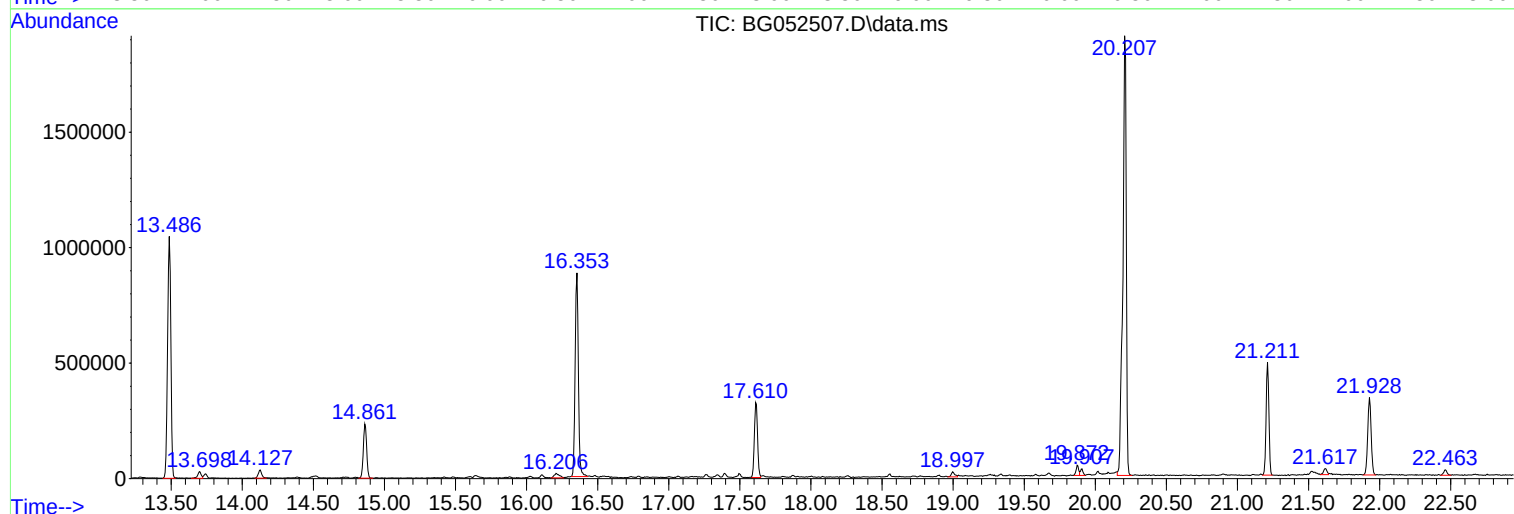
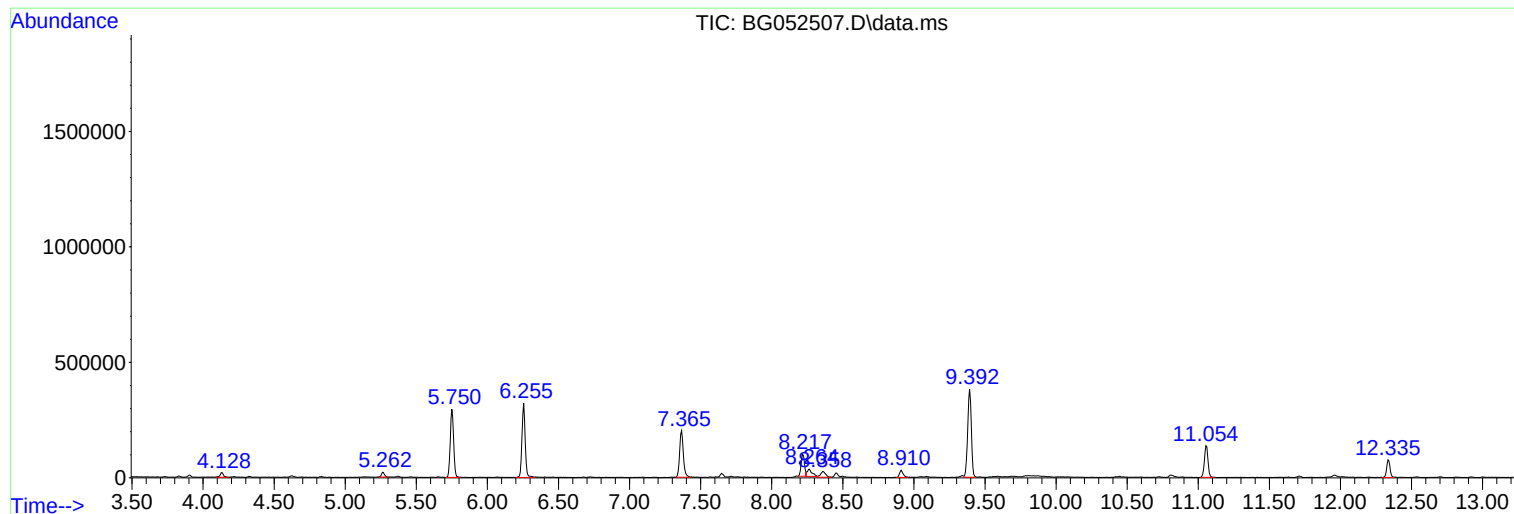
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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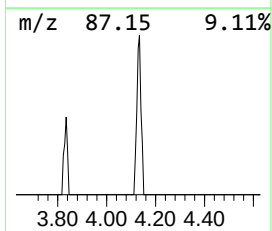
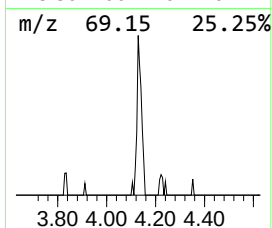
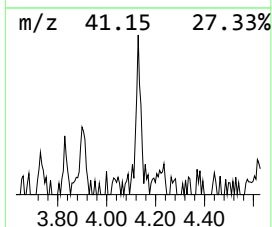
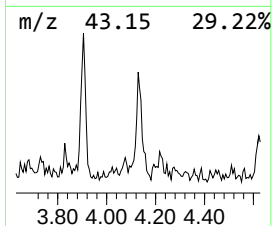
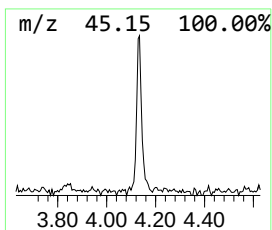
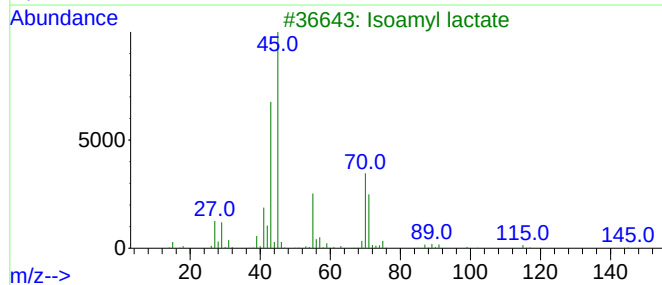
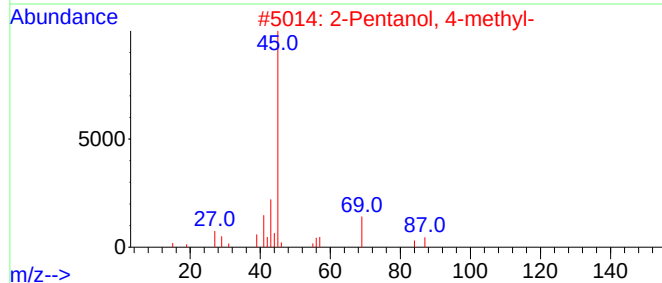
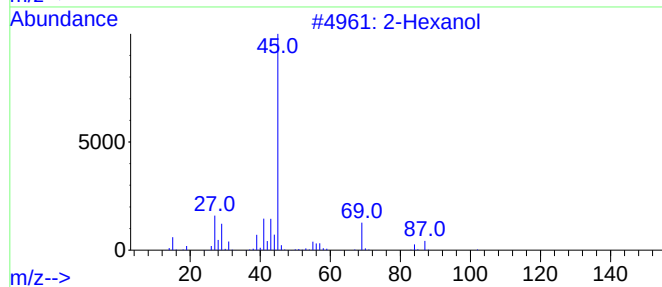
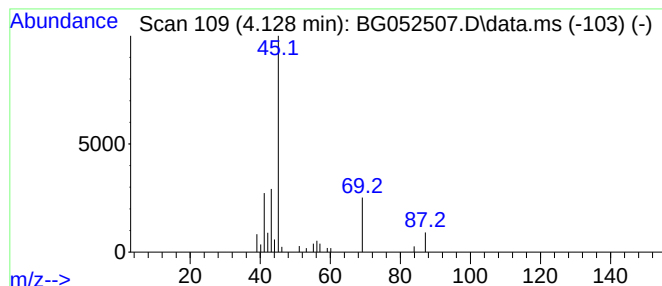
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Hexanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.128	4.41 ng	34671	1,4-Dichlorobenzene-d4	8.217

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol	102	C6H14O	000626-93-7	83
2			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	78
3			Isoamyl lactate	160	C8H16O3	019329-89-6	39
4			1-Butene, 4-methoxy	86	C5H10O	004696-30-4	39
5			Hydrazine, propyl-	74	C3H10N2	005039-61-2	38



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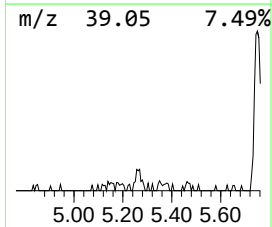
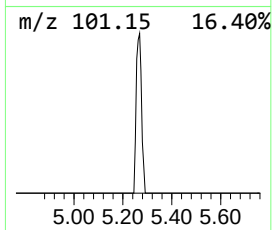
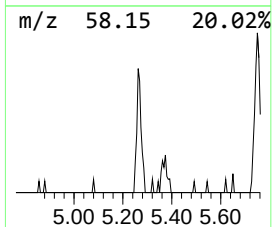
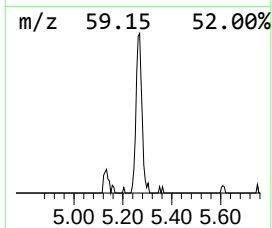
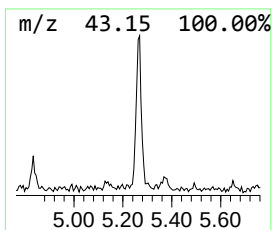
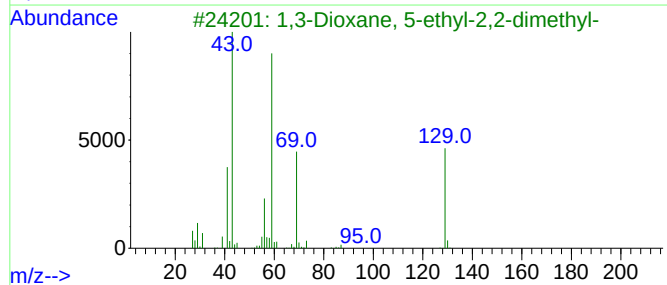
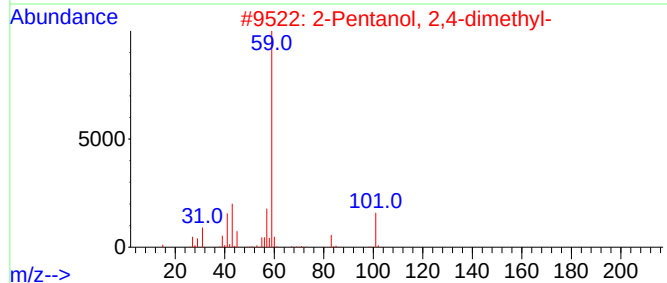
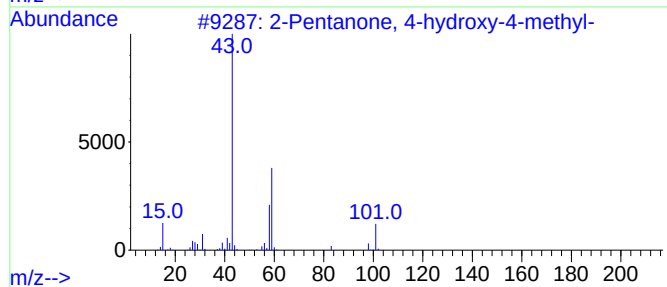
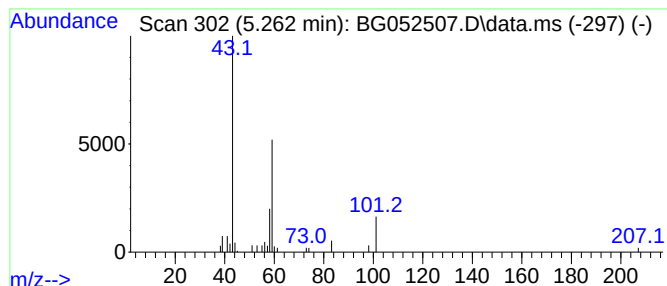
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.262	4.08 ng	32094	1,4-Dichlorobenzene-d4	8.217

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	37
3			1,3-Dioxane, 5-ethyl-2,2-dimethyl-	144	C8H16O2	025796-26-3	25
4			3-Octanol	130	C8H18O	000589-98-0	23
5			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	23



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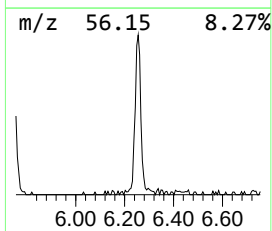
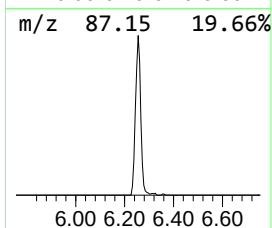
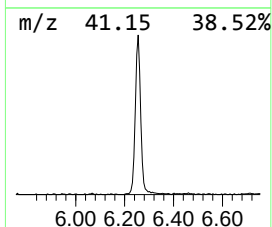
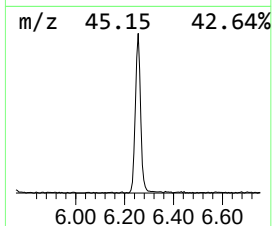
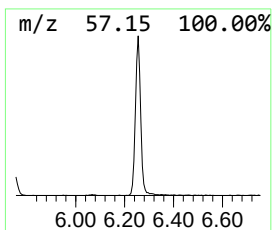
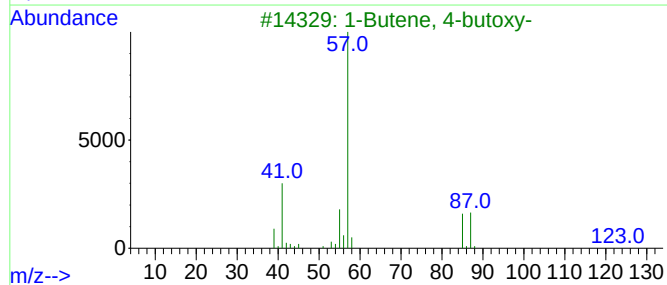
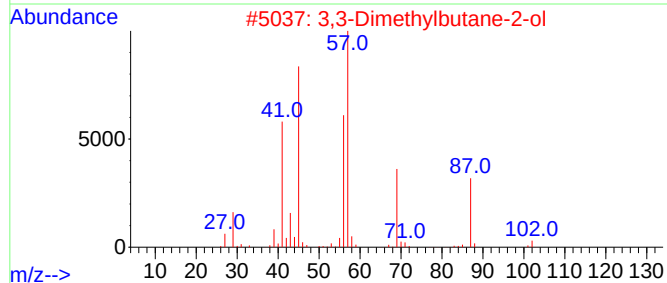
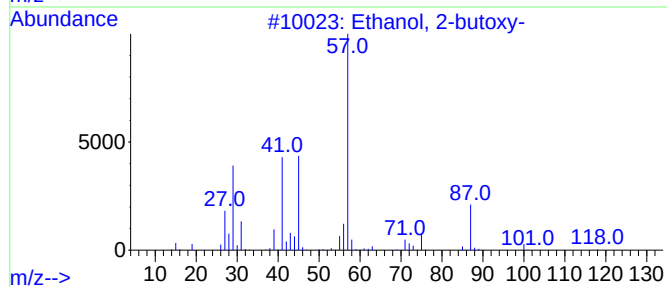
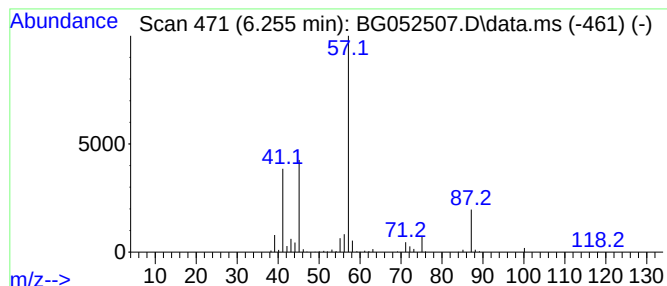
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.255	64.00 ng	503093	1,4-Dichlorobenzene-d4	8.217

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	59
3			1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	25
4			n-Butyl ether	130	C8H18O	000142-96-1	25
5			Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	17



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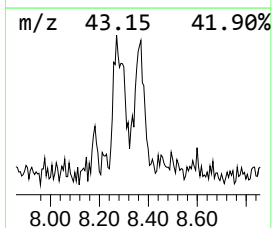
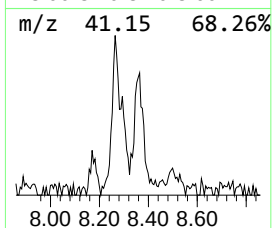
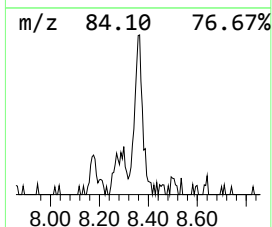
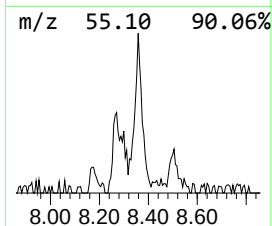
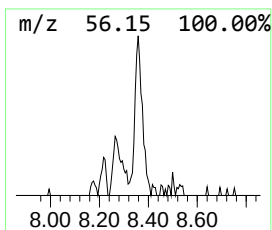
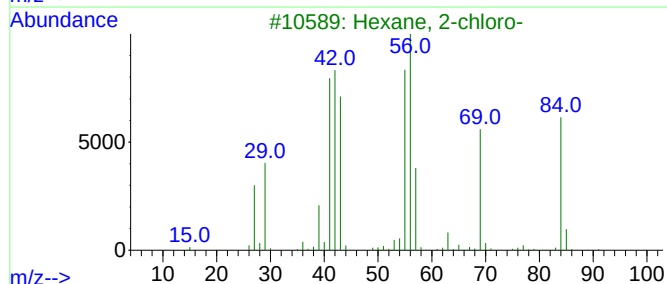
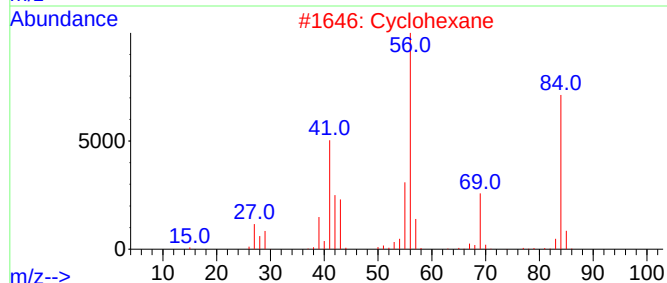
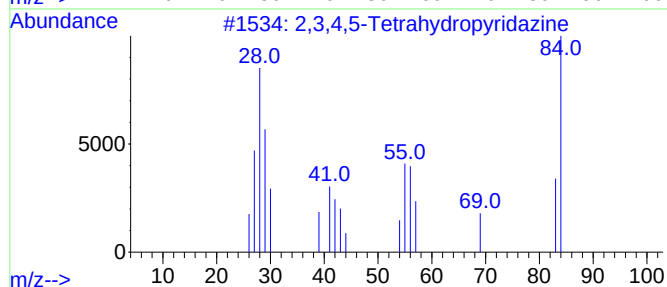
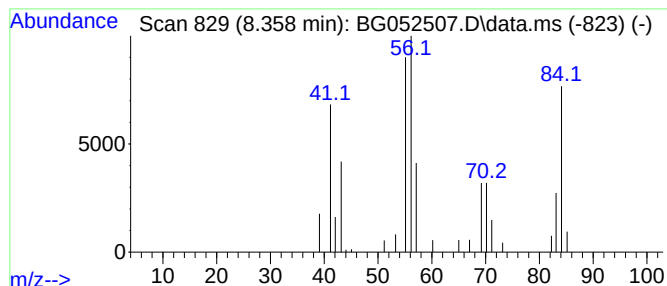
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2,3,4,5-Tetrahydropyridazine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.358	7.49 ng	58900	1,4-Dichlorobenzene-d4	8.217

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,3,4,5-Tetrahydropyridazine	84	C4H8N2	000694-06-4	64
2		Cyclohexane	84	C6H12	000110-82-7	59
3		Hexane, 2-chloro-	120	C6H13Cl	000638-28-8	45
4		Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	43
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	42



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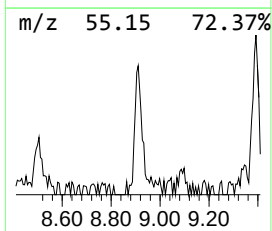
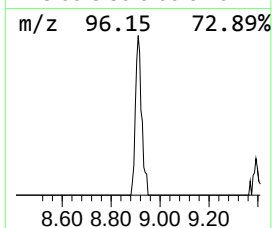
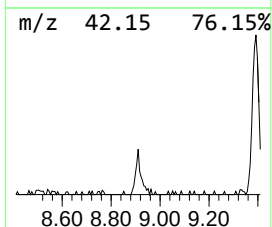
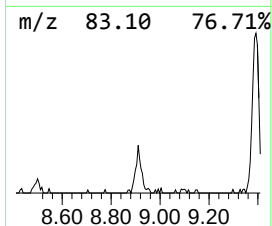
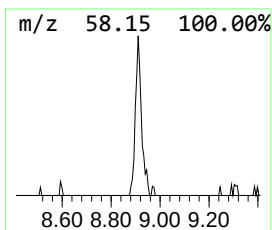
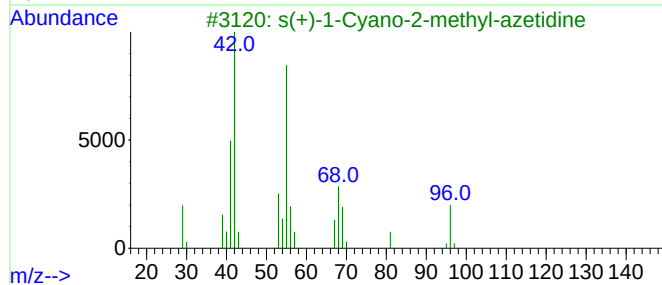
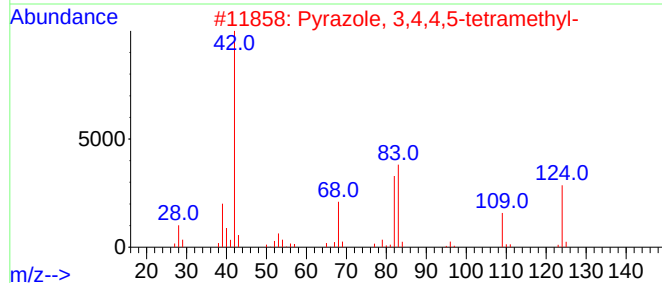
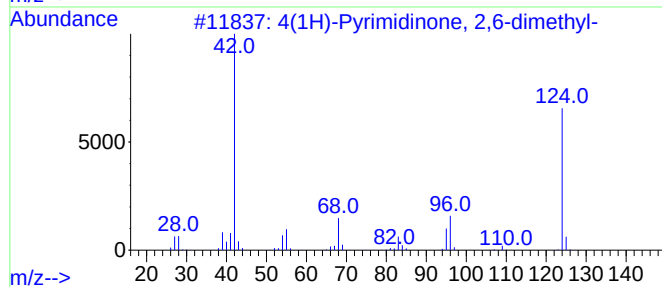
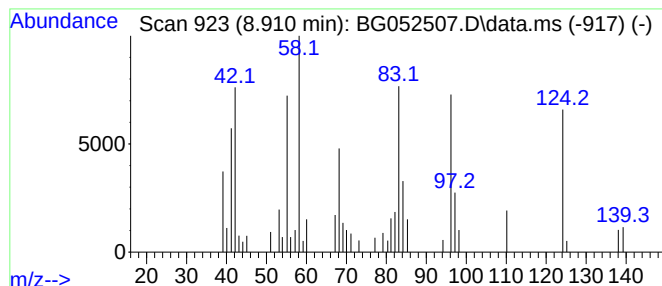
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown8.910 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.910	7.00 ng	55030	1,4-Dichlorobenzene-d4	8.217

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4(1H)-Pyrimidinone, 2,6-dimethyl-	124	C6H8N2O	006622-92-0	38
2			Pyrazole, 3,4,4,5-tetramethyl-	124	C7H12N2	019078-32-1	37
3			s(+)-1-Cyano-2-methyl-azetidine	96	C5H8N2	1000143-32-0	25
4			Ethanethiol, 2-(dimethylamino)-	105	C4H11NS	000108-02-1	22
5			Nonenyl angelate, 3Z-	224	C14H24O2	1000383-61-4	16



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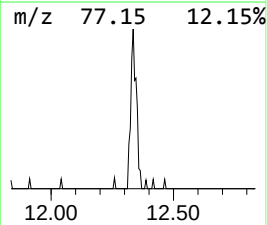
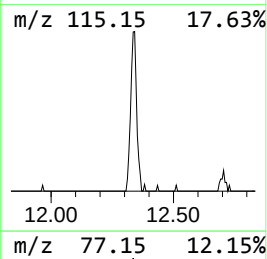
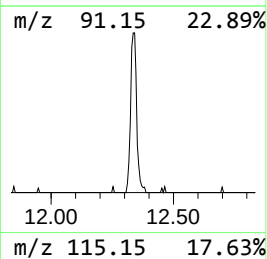
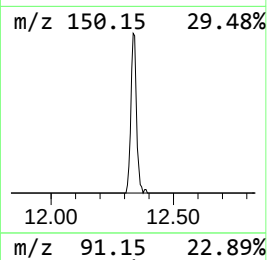
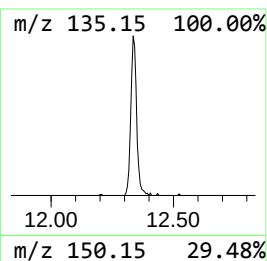
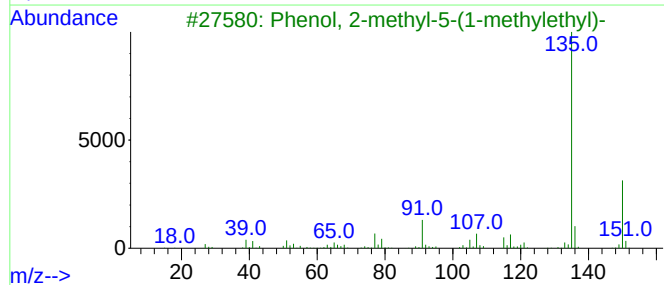
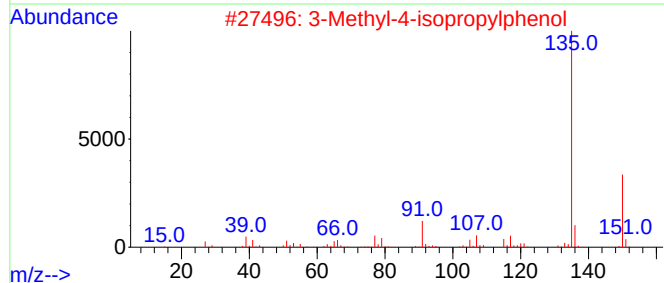
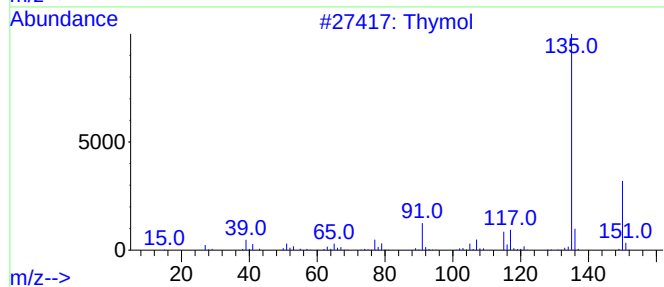
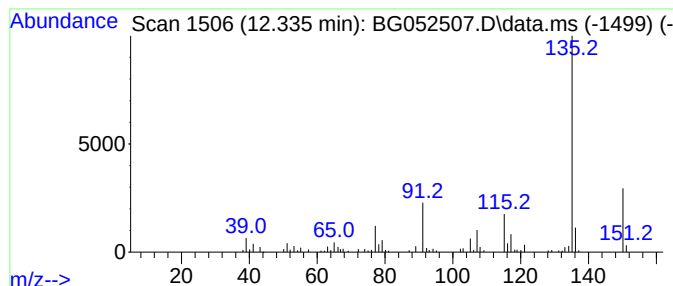
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Thymol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.335	10.60 ng	126584	Naphthalene-d8	11.054

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thymol	150	C10H14O	000089-83-8	90
2			3-Methyl-4-isopropylphenol	150	C10H14O	003228-02-2	90
3			Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	87
4			Phenol, 2,3,4,6-tetramethyl-	150	C10H14O	003238-38-8	80
5			Phenol, 2,3,5,6-tetramethyl-	150	C10H14O	000527-35-5	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022822\
Data File : BG052507.D
Acq On : 28 Feb 2022 18:44
Operator : CG/JU
Sample : N1668-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PURGED-WATER

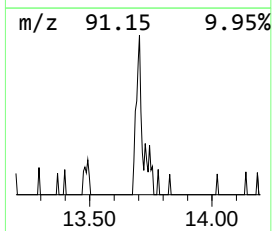
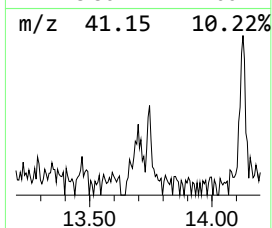
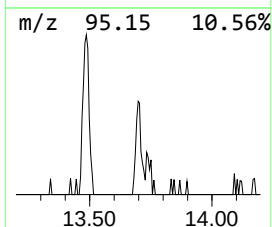
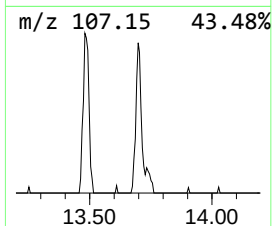
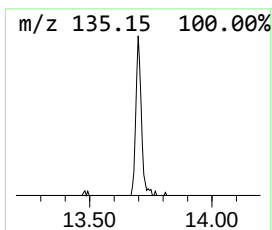
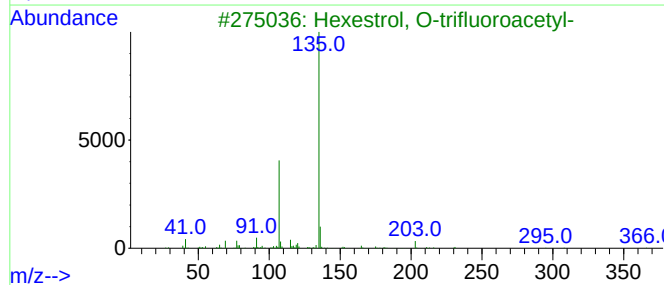
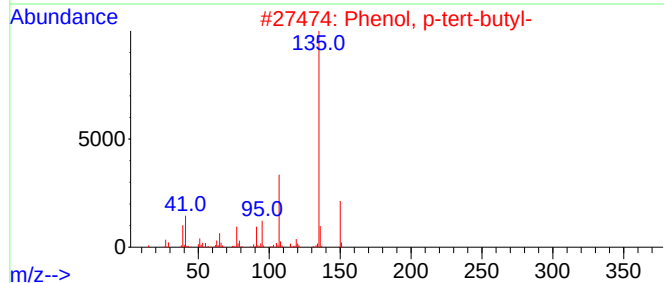
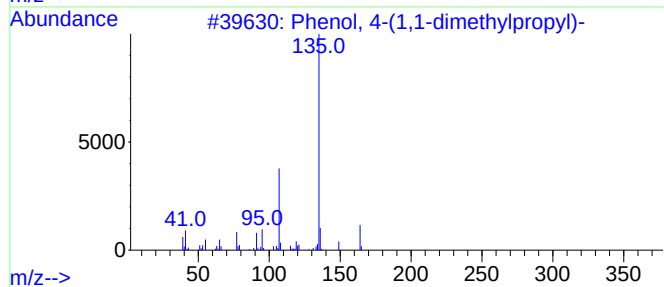
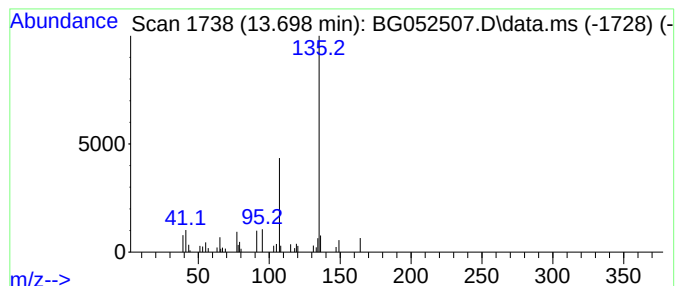
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.698	2.72 ng	51738	Acenaphthene-d10	14.861

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	80
2		Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	72
3		Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	64
4		Hexestrol, O-(n-propyloxycarbonyl)-	356	C22H28O4	1000487-65-1	59
5		4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022822\
Data File : BG052507.D
Acq On : 28 Feb 2022 18:44
Operator : CG/JU
Sample : N1668-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PURGED-WATER

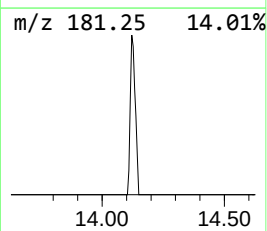
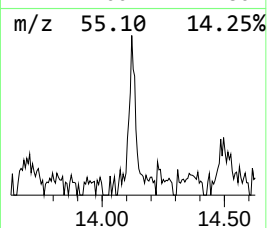
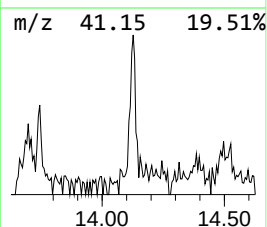
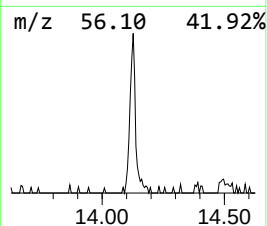
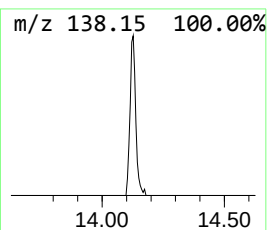
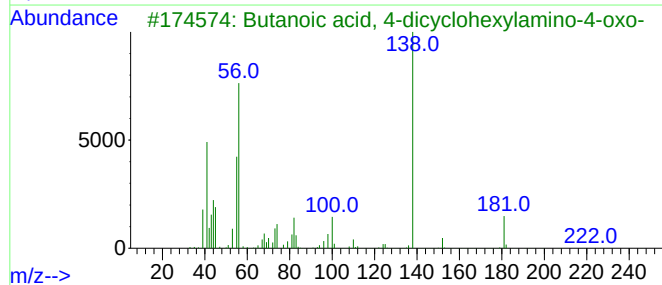
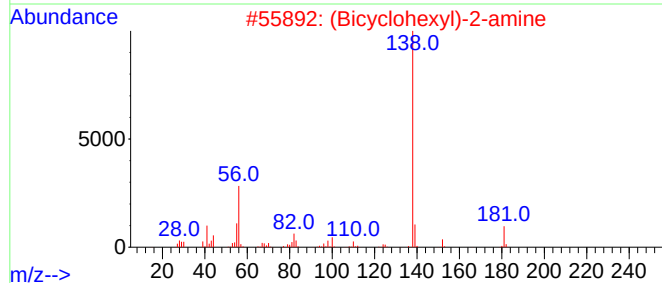
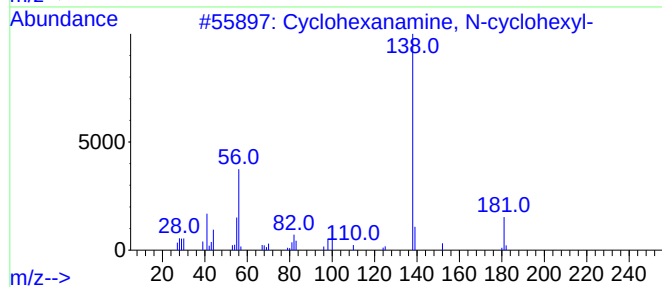
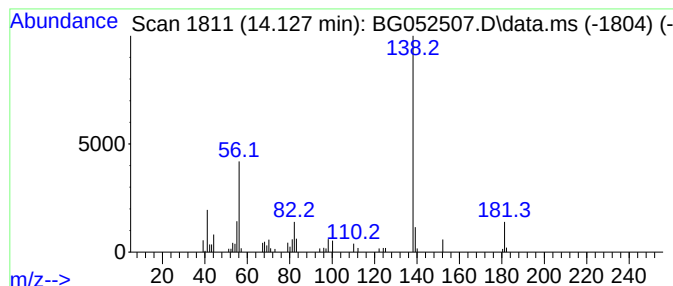
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexanamine, N-cyclohexyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.127	3.12 ng	59348	Acenaphthene-d10	14.861

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	97
2			(Bicyclohexyl)-2-amine	181	C12H23N	006283-14-3	95
3			Butanoic acid, 4-dicyclohexylami...	281	C16H27NO3	328013-95-2	64
4			Gephyrotoxin 181b	181	C12H23N	120030-08-2	47
5			4,6-Dimethyl-2-pyrimidinylhydrazine	138	C6H10N4	023906-13-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022822\
Data File : BG052507.D
Acq On : 28 Feb 2022 18:44
Operator : CG/JU
Sample : N1668-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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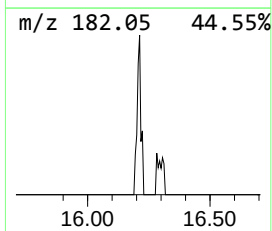
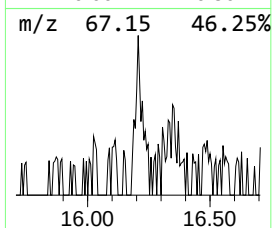
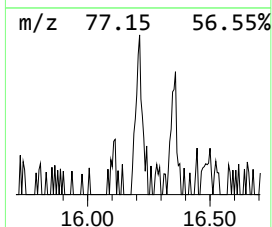
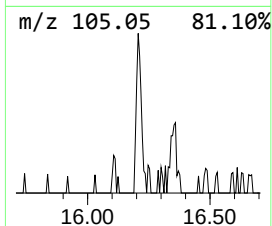
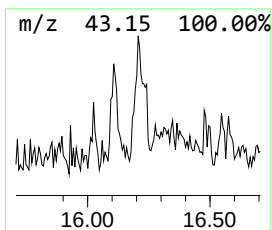
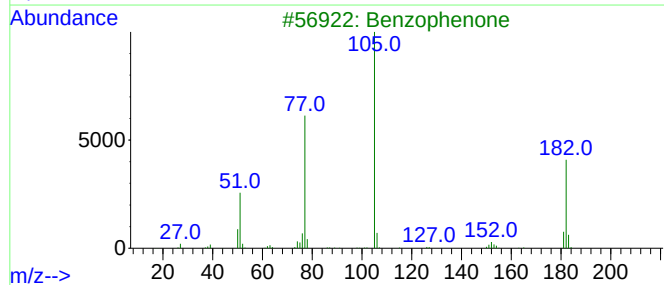
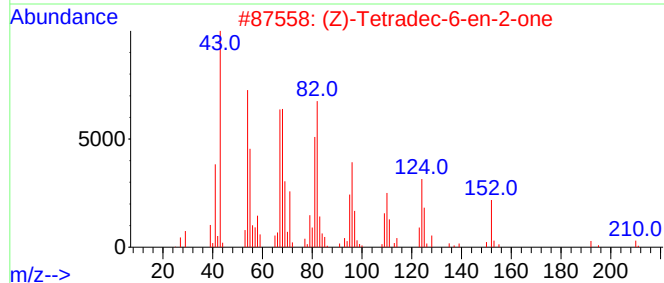
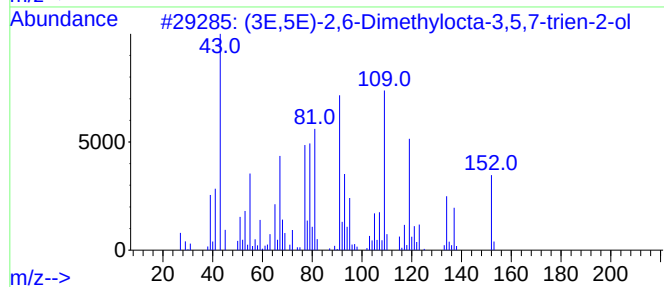
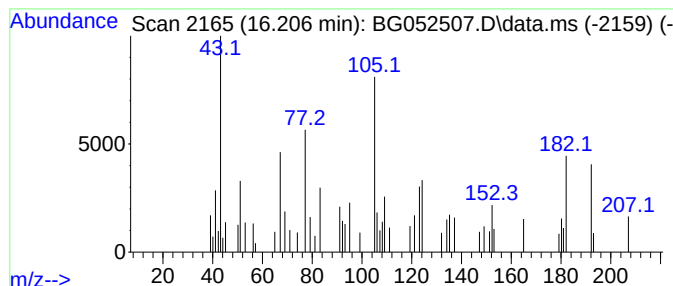
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.206 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.206	2.52 ng	47881	Acenaphthene-d10	14.861

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(3E,5E)-2,6-Dimethylocta-3,5,7-t...	152	C10H16O	206115-88-0	35
2		(Z)-Tetradec-6-en-2-one	210	C14H26O	1000466-27-1	16
3		Benzophenone	182	C13H10O	000119-61-9	14
4		2-Methyl-5-nitrophenol	153	C7H7NO3	005428-54-6	11
5		Benzene, nitro-	123	C6H5NO2	000098-95-3	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022822\
Data File : BG052507.D
Acq On : 28 Feb 2022 18:44
Operator : CG/JU
Sample : N1668-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PURGED-WATER

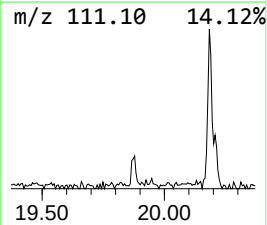
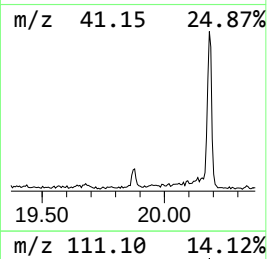
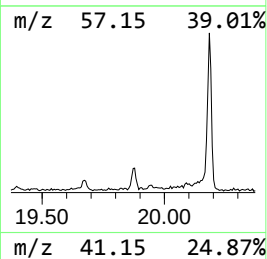
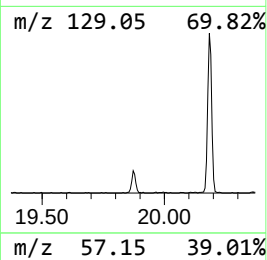
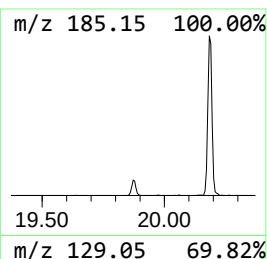
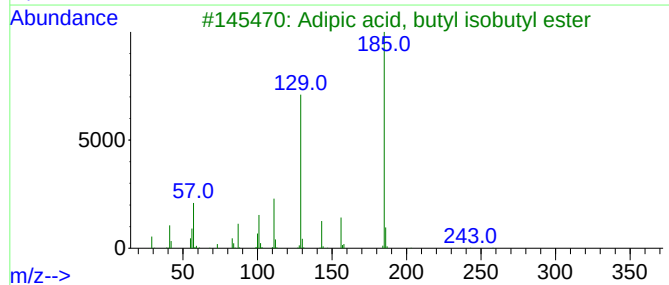
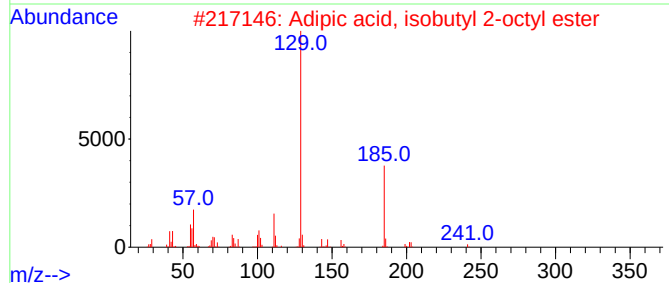
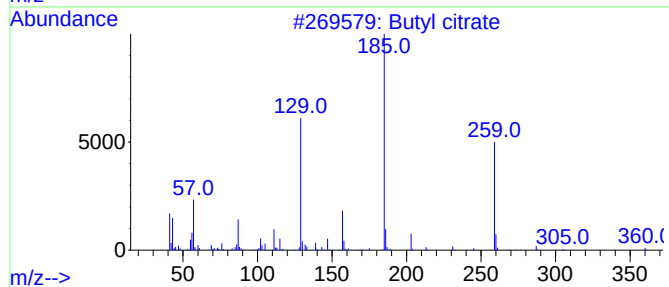
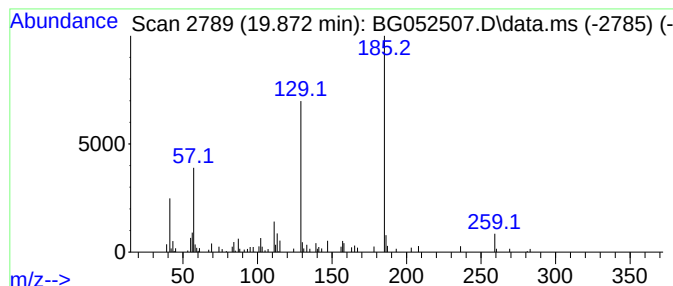
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Butyl citrate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.872	2.07 ng	57920	Chrysene-d12	21.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	78
2			Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	72
3			Adipic acid, butyl isobutyl ester	258	C14H26O4	1010324-09-3	72
4			Adipic acid, butyl 4-heptyl ester	300	C17H32O4	1000349-73-7	64
5			1-Cyano-4-cyclohexylbenzene	185	C13H15N	027634-88-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022822\
Data File : BG052507.D
Acq On : 28 Feb 2022 18:44
Operator : CG/JU
Sample : N1668-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PURGED-WATER

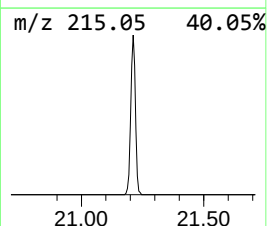
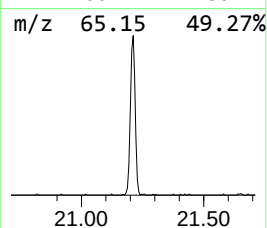
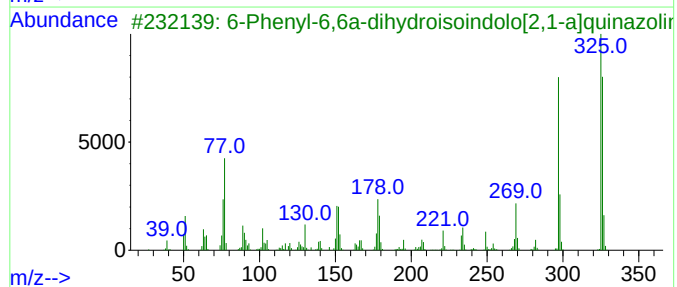
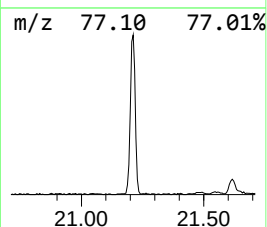
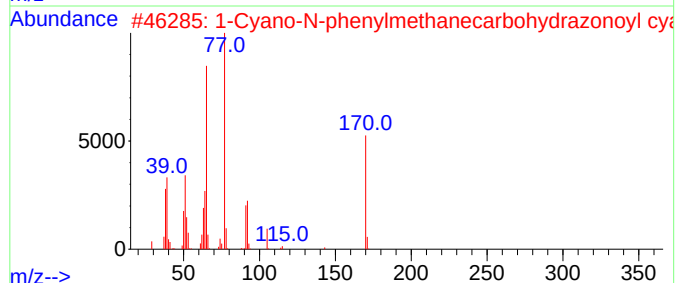
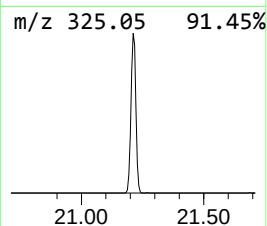
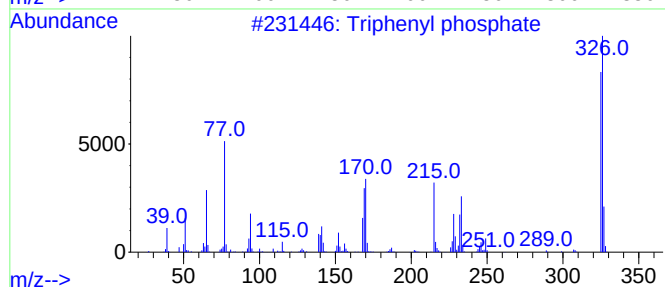
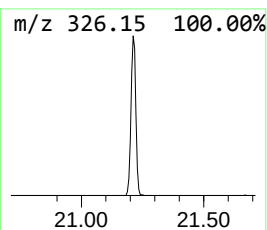
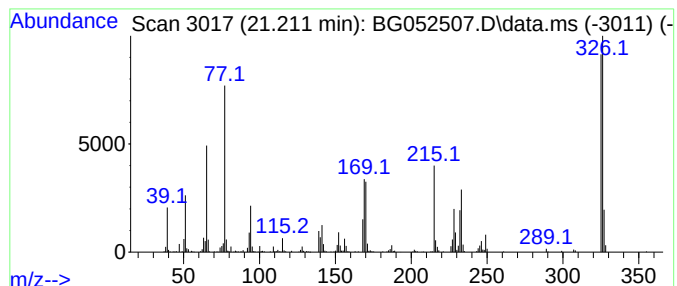
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Triphenyl phosphate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.211	23.92 ng	668876	Chrysene-d12	21.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenyl phosphate	326	C18H15O4P	000115-86-6	99
2			1-Cyano-N-phenylmethanecarbohydr...	170	C9H6N4	000306-18-3	38
3			6-Phenyl-6,6a-dihydroisindolo[2...	326	C21H14N2O2	1000482-29-8	25
4			Coumarin, 3-benzoyl-4-phenyl-	326	C22H14O3	019725-29-2	25
5			Pyrazol-5-amine, 3-(4-chlorophen...	326	C16H11ClN4S	1000271-07-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022822\
Data File : BG052507.D
Acq On : 28 Feb 2022 18:44
Operator : CG/JU
Sample : N1668-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PURGED-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.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
2-Hexanol	4.128	4.4	ng	34671	1	8.217	157228	20.0
2-Pentanone, 4-...	5.262	4.1	ng	32094	1	8.217	157228	20.0
Ethanol, 2-butoxy-	6.255	64.0	ng	503093	1	8.217	157228	20.0
2,3,4,5-Tetrahy...	8.358	7.5	ng	58900	1	8.217	157228	20.0
unknown8.910	8.910	7.0	ng	55030	1	8.217	157228	20.0
Thymol	12.335	10.6	ng	126584	2	11.054	238759	20.0
Phenol, 4-(1,1-...	13.698	2.7	ng	51738	3	14.861	380761	20.0
Cyclohexanamine...	14.127	3.1	ng	59348	3	14.861	380761	20.0
unknown16.206	16.206	2.5	ng	47881	3	14.861	380761	20.0
Butyl citrate	19.872	2.1	ng	57920	5	21.928	559358	20.0
Triphenyl phosph...	21.211	23.9	ng	668876	5	21.928	559358	20.0