

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
 Data File : BG053338.D
 Acq On : 27 Apr 2022 2:39
 Operator : CG/JU
 Sample : N2482-19
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EB-2022-04-19

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-BG040822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053338.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.668	382	388	396	rBV	128578	217141	9.10%	2.308%
2	7.265	654	660	672	rBV	79724	151315	6.34%	1.609%
3	8.105	796	803	808	rBV	65240	114867	4.81%	1.221%
4	8.158	808	812	819	rVB3	14560	24810	1.04%	0.264%
5	9.263	993	1000	1013	rVB	222495	408631	17.13%	4.344%
6	9.427	1022	1028	1033	rBV3	20296	40141	1.68%	0.427%
7	10.678	1233	1241	1249	rBV4	17390	36073	1.51%	0.383%
8	10.913	1274	1281	1289	rBV2	86490	161860	6.78%	1.721%
9	11.272	1336	1342	1349	rBV4	13097	27810	1.17%	0.296%
10	11.830	1428	1437	1445	rVB4	11844	28248	1.18%	0.300%
11	13.087	1645	1651	1660	rBV2	52348	90135	3.78%	0.958%
12	13.351	1685	1696	1705	rBV	625174	1101121	46.15%	11.706%
13	13.569	1726	1733	1741	rBV	524071	796987	33.41%	8.473%
14	13.645	1741	1746	1754	rVB2	43736	75542	3.17%	0.803%
15	14.726	1924	1930	1936	rBV	158335	250961	10.52%	2.668%
16	15.014	1973	1979	1988	rVB	102036	165023	6.92%	1.754%
17	15.137	1994	2000	2005	rBV3	25476	35108	1.47%	0.373%
18	15.454	2048	2054	2060	rVB	193354	273210	11.45%	2.904%
19	15.525	2060	2066	2072	rVB	60373	88544	3.71%	0.941%
20	16.065	2152	2158	2167	rBV	54616	87524	3.67%	0.930%
21	16.212	2176	2183	2196	rBV	584760	948454	39.75%	10.083%
22	16.800	2277	2283	2291	rBV	178221	284537	11.93%	3.025%
23	17.475	2391	2398	2405	rBV	244053	382969	16.05%	4.071%
24	18.127	2503	2509	2514	rBV2	113289	151897	6.37%	1.615%
25	20.078	2835	2841	2851	rVB	1783064	2385759	100.00%	25.362%
26	21.752	3120	3126	3133	rBV	308007	519624	21.78%	5.524%
27	23.244	3374	3380	3389	rBV10	14918	38300	1.61%	0.407%
28	25.047	3677	3687	3698	rVB2	177604	520123	21.80%	5.529%

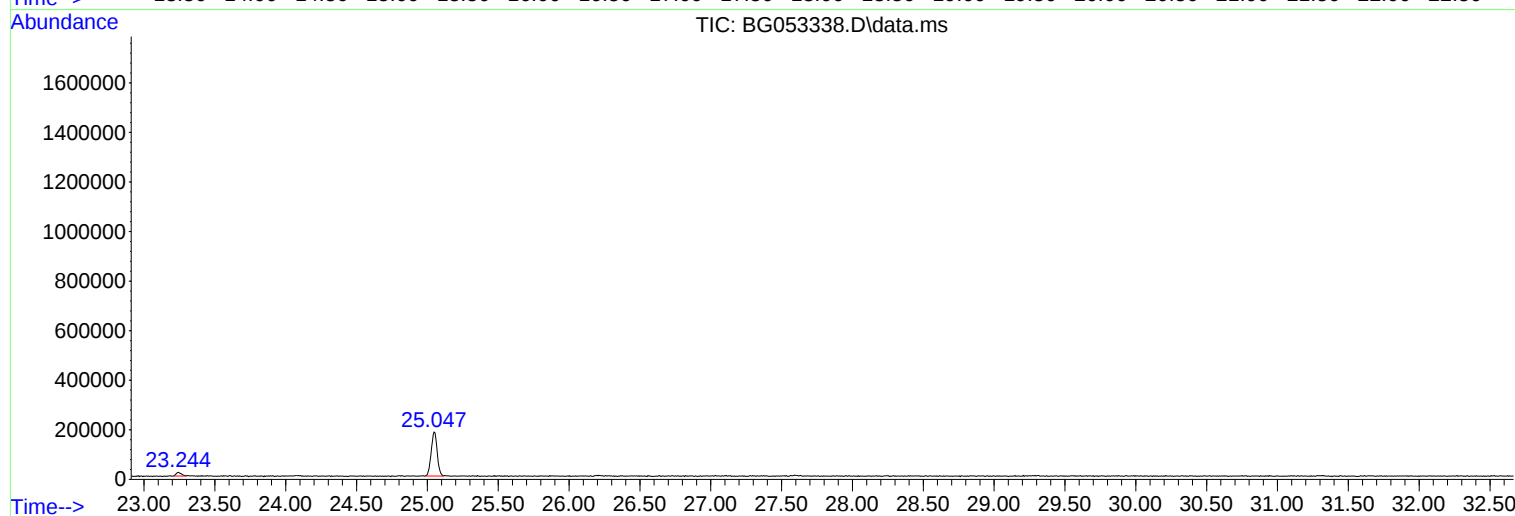
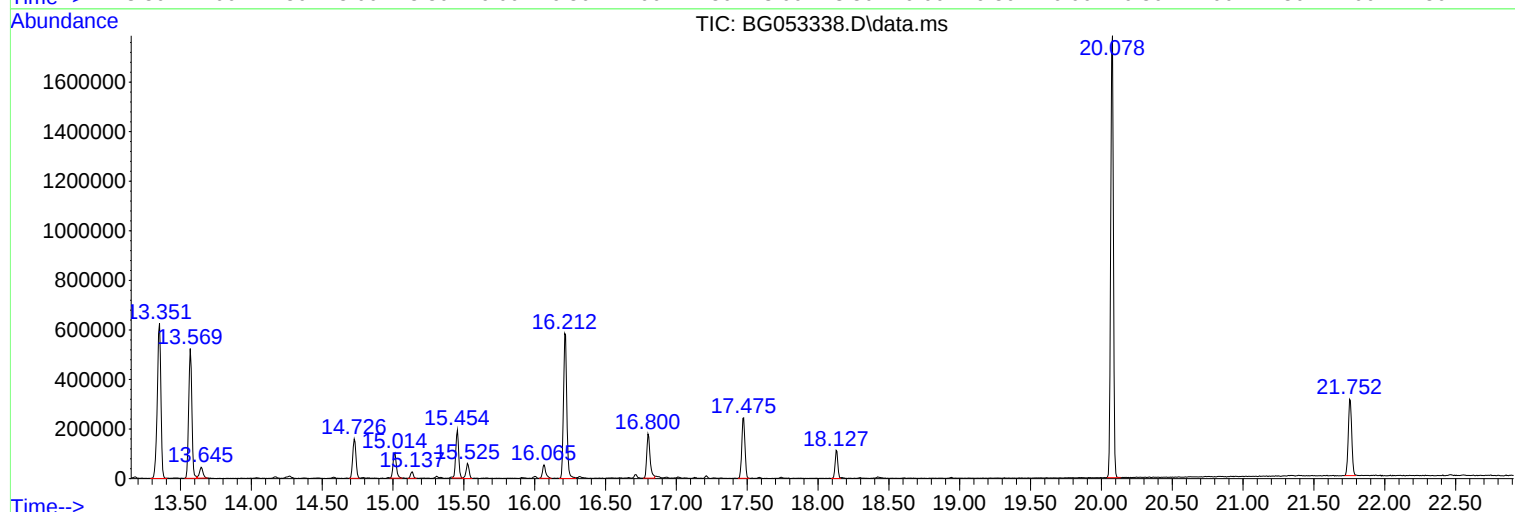
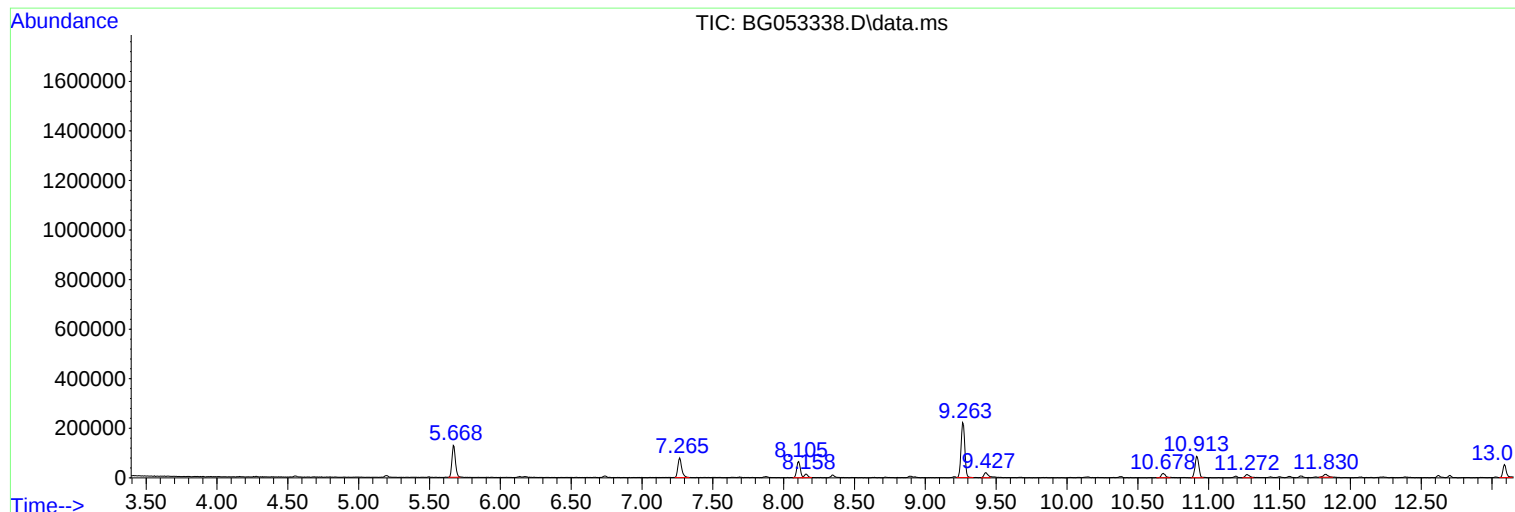
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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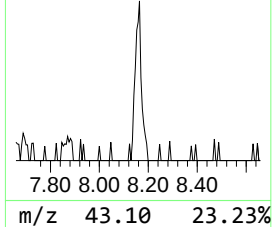
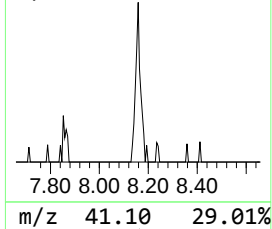
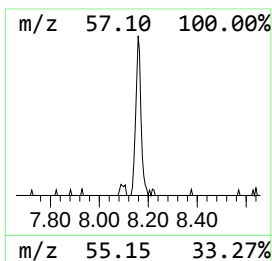
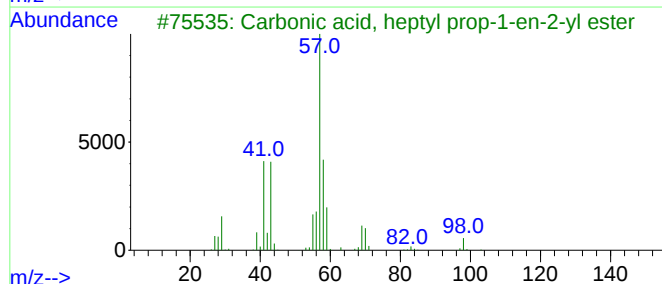
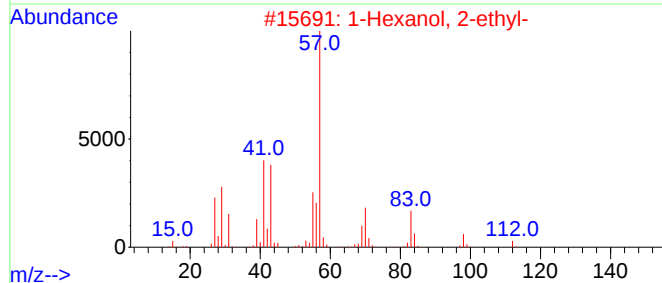
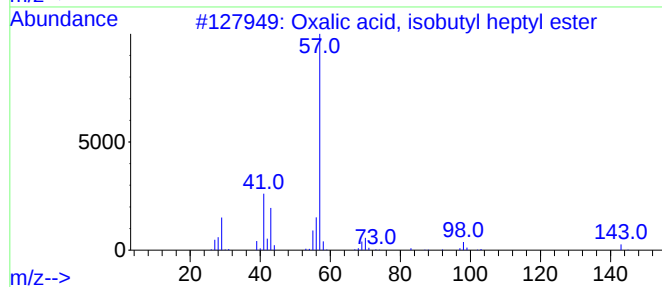
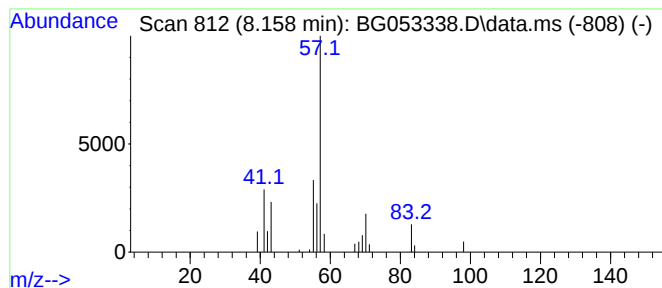
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Oxalic acid, isobutyl heptyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.158	4.32 ng	24810	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	53
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
3			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	39
4			Acetic acid, dichloro-, heptyl e...	226	C9H16Cl2O2	083004-97-1	38
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	38



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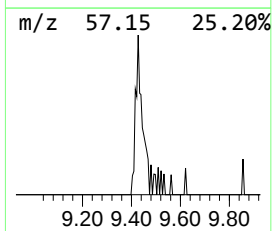
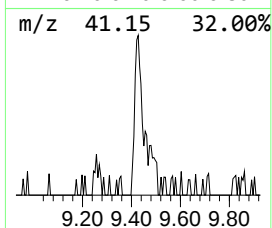
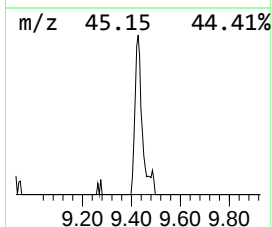
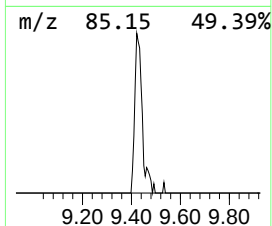
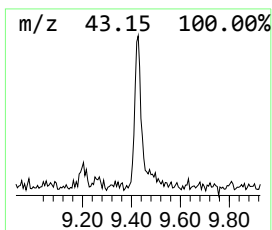
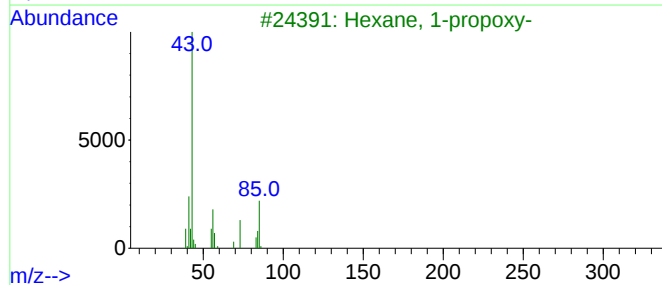
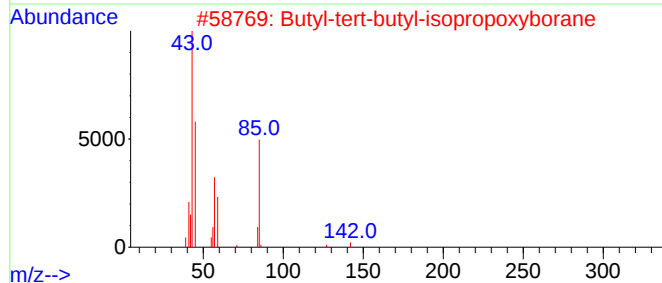
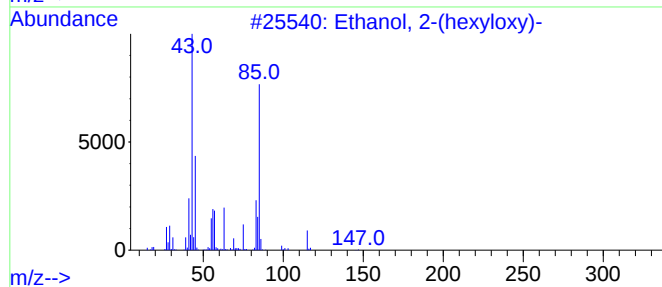
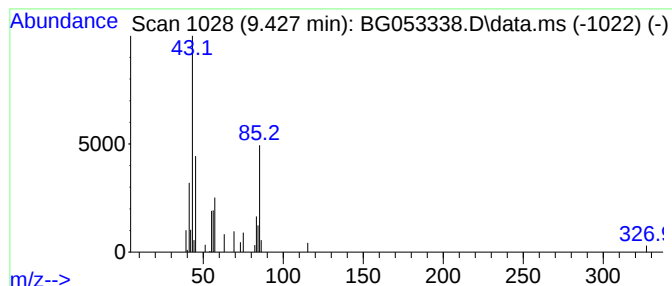
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Peak Number 2 Ethanol, 2-(hexyloxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.427	6.99 ng	40141	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(hexyloxy)-	146	C8H18O2	000112-25-4	72
2			Butyl-tert-butyl-isopropoxyborane	184	C11H25BO	097782-82-6	47
3			Hexane, 1-propoxy-	144	C9H20O	053685-78-2	43
4			Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	38
5			Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	38



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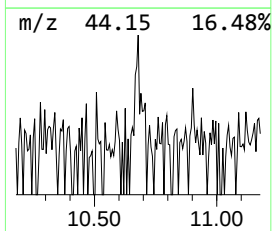
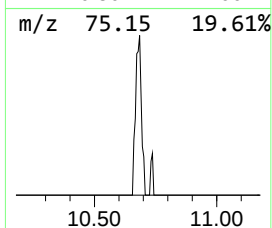
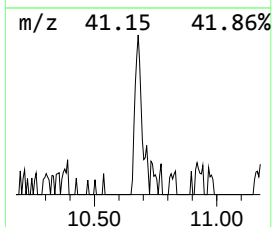
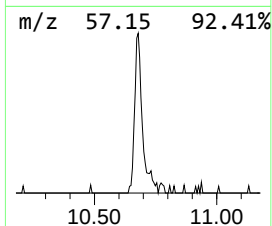
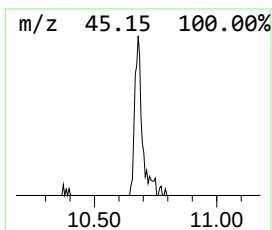
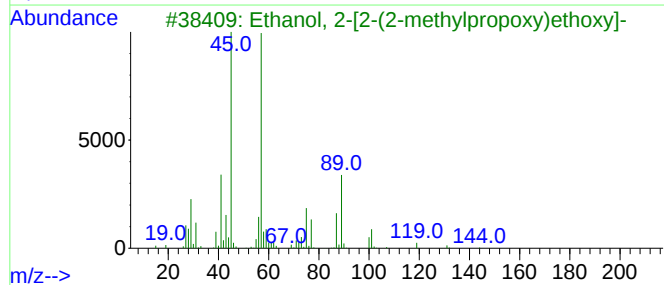
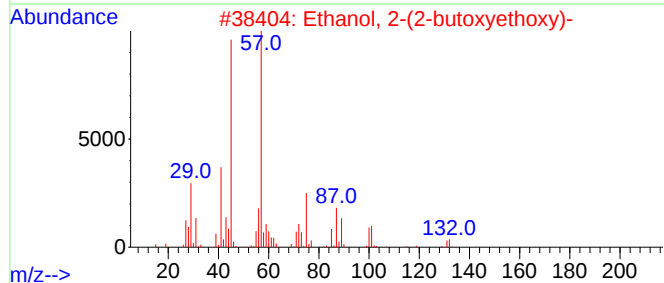
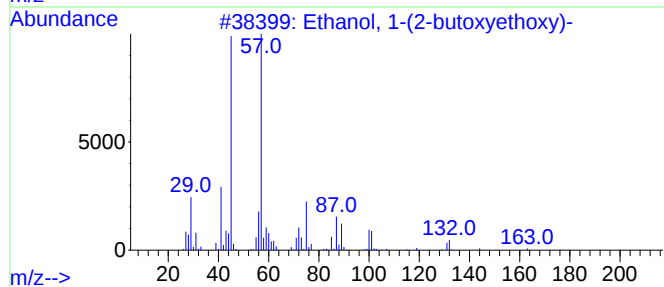
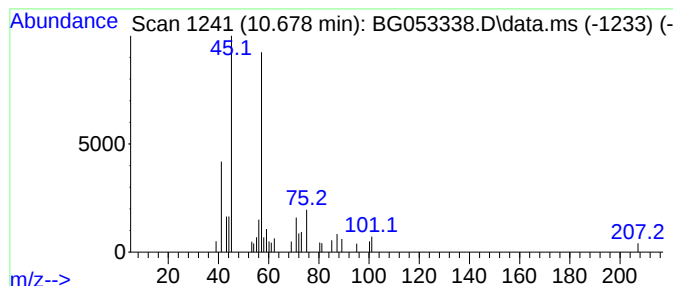
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.679	4.46 ng	36073	Naphthalene-d8	10.913	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	86
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	45
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	42



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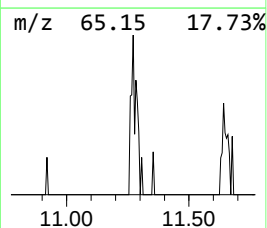
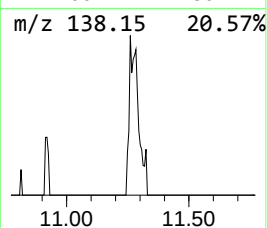
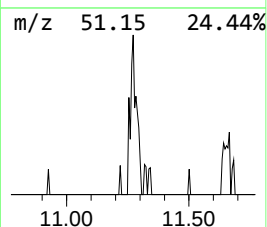
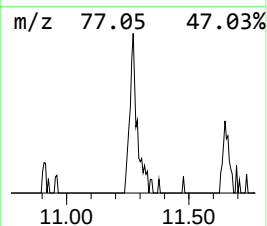
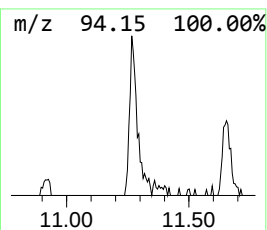
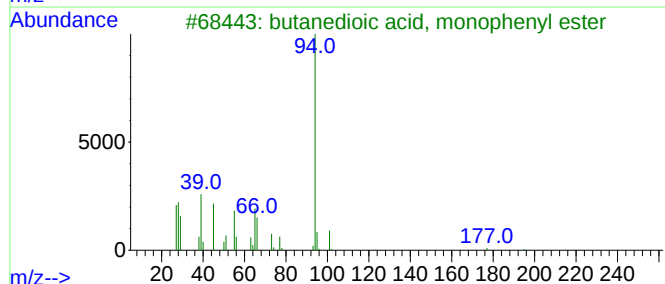
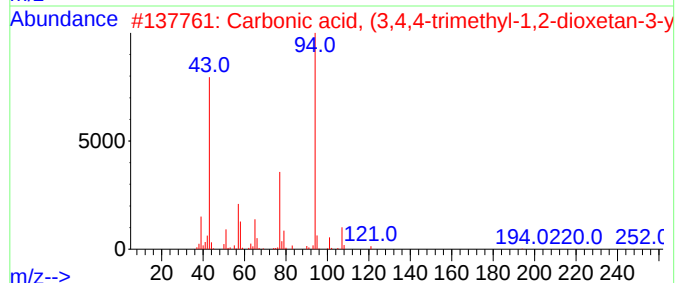
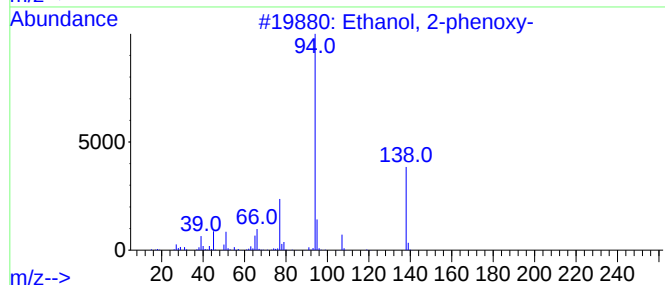
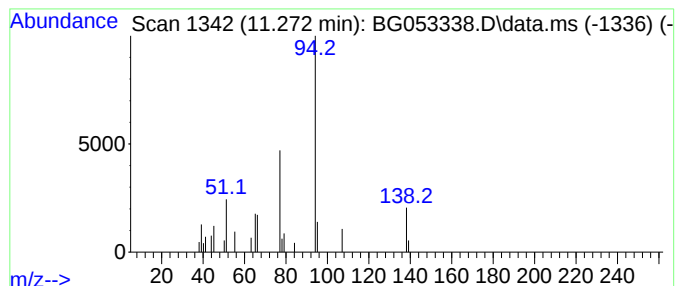
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Ethanol, 2-phenoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.272	3.44 ng	27810	Naphthalene-d8	10.913

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	91
2			Carbonic acid, (3,4,4-trimethyl-...	252	C13H16O5	109123-69-5	45
3			butanedioic acid, monophenyl ester	194	C10H10O4	1000400-29-4	43
4			Phenol	94	C6H6O	000108-95-2	43
5			2-Pyridinecarboxylic acid, 3-amino-	138	C6H6N2O2	001462-86-8	38



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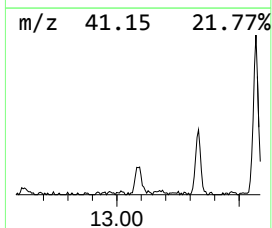
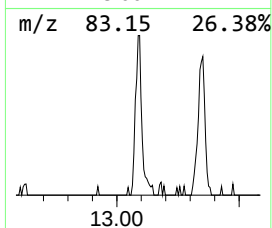
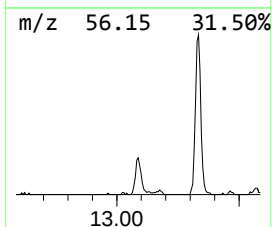
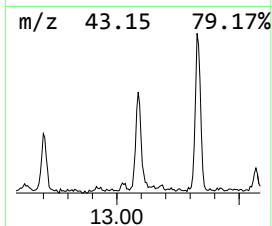
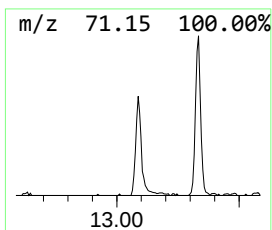
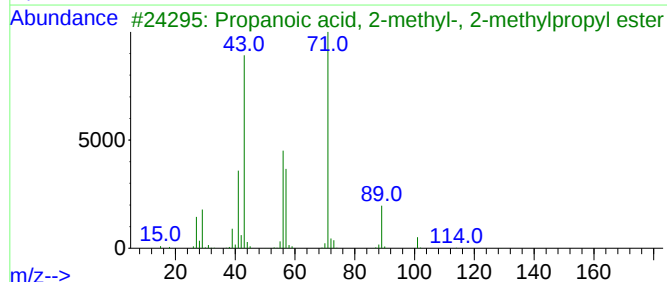
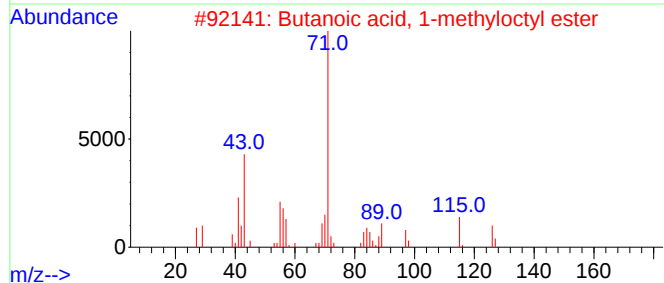
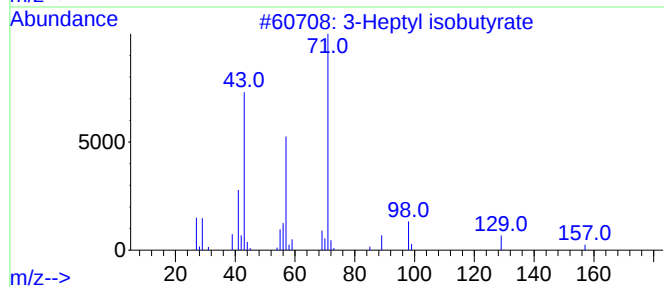
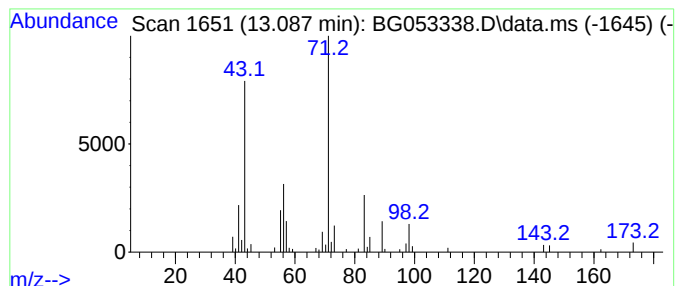
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Peak Number 5 3-Heptyl isobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.087	7.18 ng	90135	Acenaphthene-d10	14.726

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptyl isobutyrate	186	C11H22O2	1000430-90-3	53
2			Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	53
3			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	53
4			3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	47
5			3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	45



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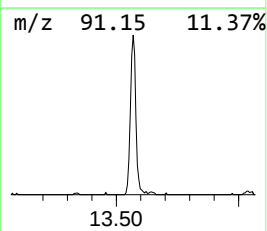
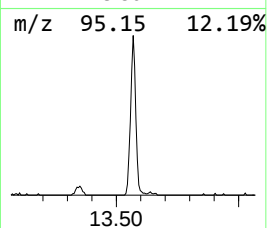
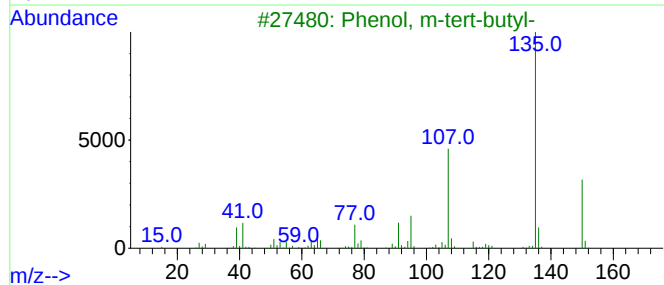
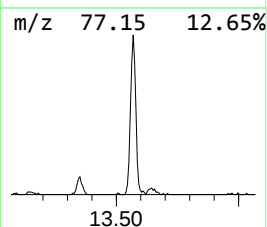
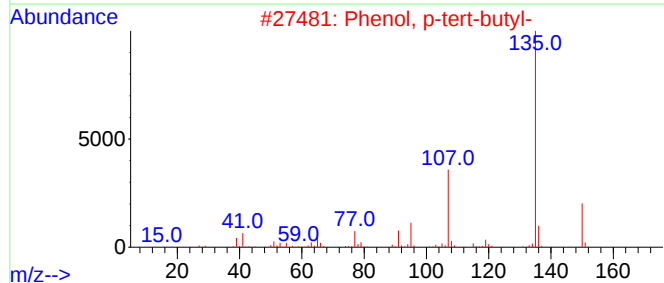
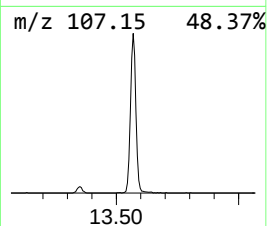
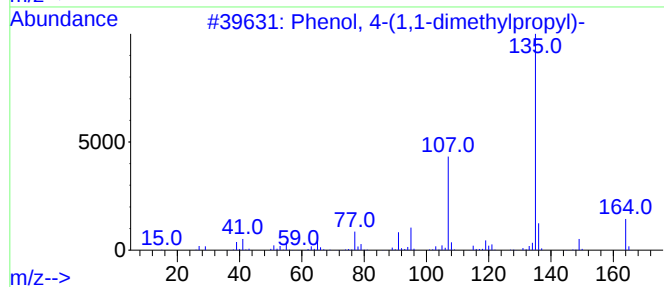
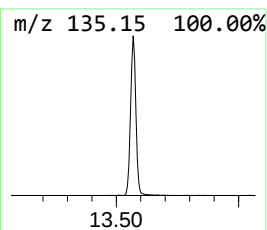
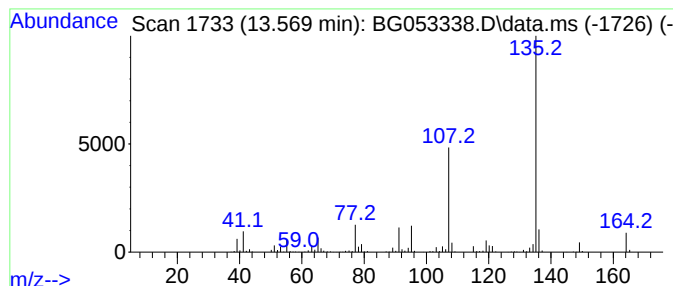
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ClientSampleId :
EB-2022-04-19

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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 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.569	63.51 ng	796987	Acenaphthene-d10		14.726	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-		164	C11H16O	000080-46-6	96
2	Phenol, p-tert-butyl-		150	C10H14O	000098-54-4	90
3	Phenol, m-tert-butyl-		150	C10H14O	000585-34-2	78
4	Imidazo[1,2-c]pyrimidin-5-ol		135	C6H5N3O	055662-66-3	64
5	Hexestrol		270	C18H22O2	000084-16-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053338.D
Acq On : 27 Apr 2022 2:39
Operator : CG/JU
Sample : N2482-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EB-2022-04-19

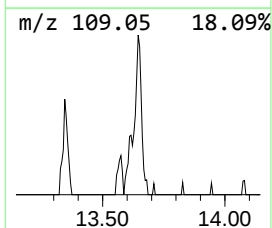
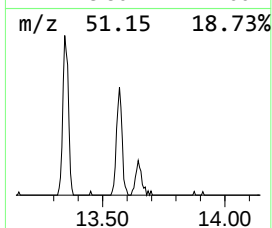
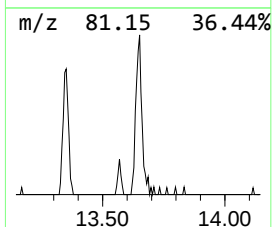
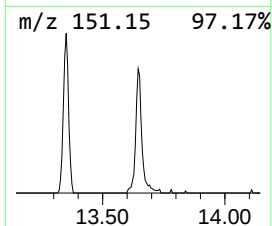
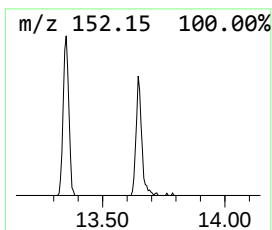
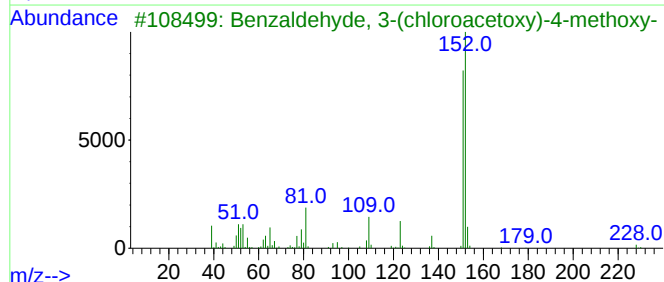
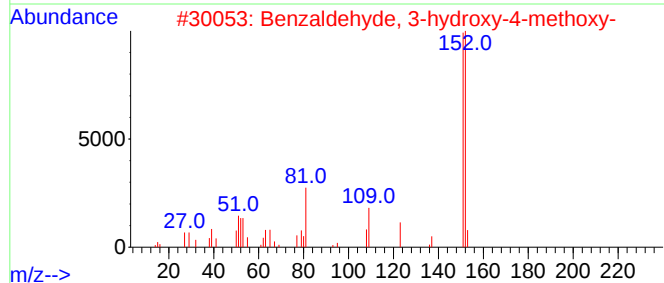
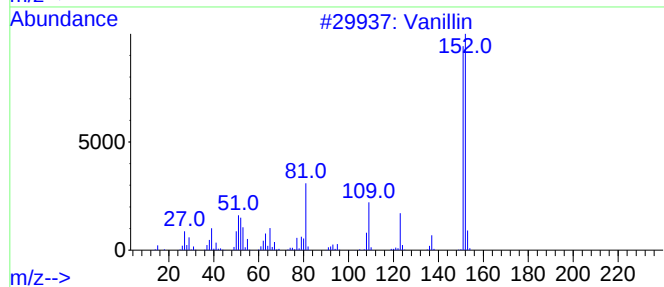
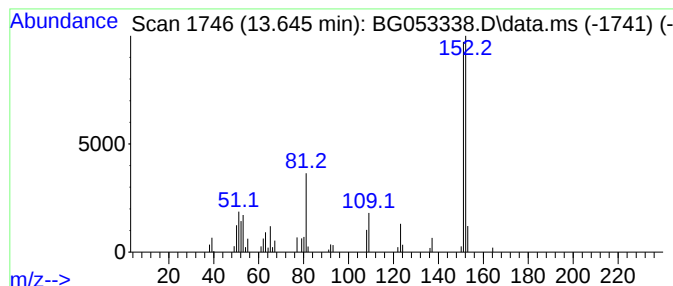
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Vanillin Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.645	6.02 ng	75542	Acenaphthene-d10	14.726

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vanillin	152	C8H8O3	000121-33-5	97
2			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96
3			Benzaldehyde, 3-(chloroacetoxy)-...	228	C10H9ClO4	066267-38-7	86
4			Benzaldehyde, 4-(methylthio)-	152	C8H8OS	003446-89-7	80
5			Vanillin lactoside	476	C20H28O13	1000129-94-7	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053338.D
Acq On : 27 Apr 2022 2:39
Operator : CG/JU
Sample : N2482-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

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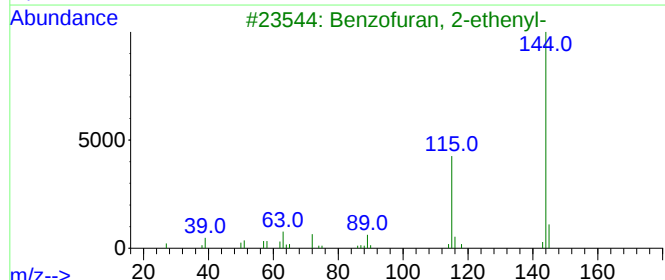
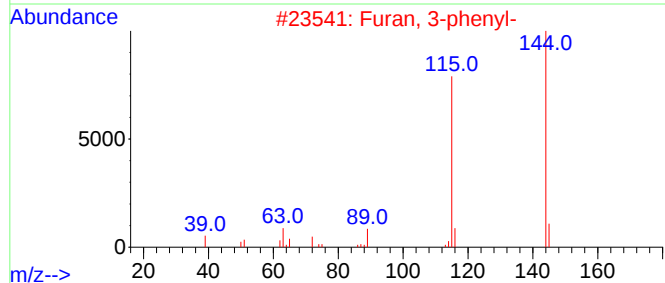
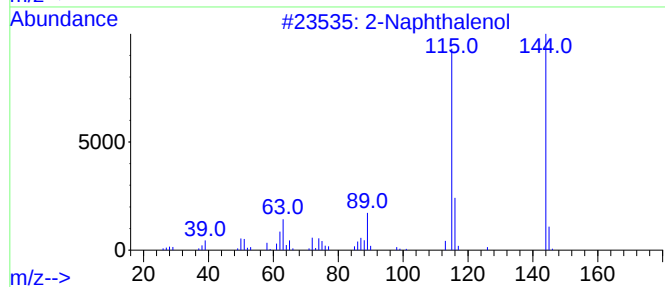
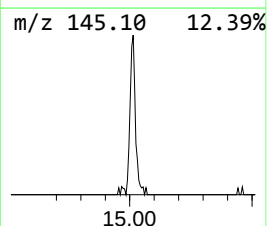
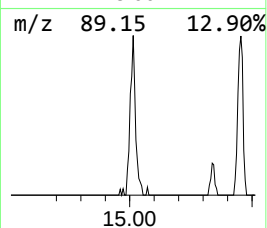
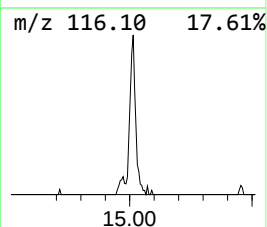
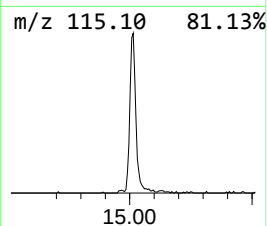
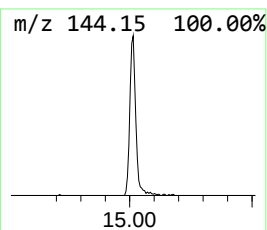
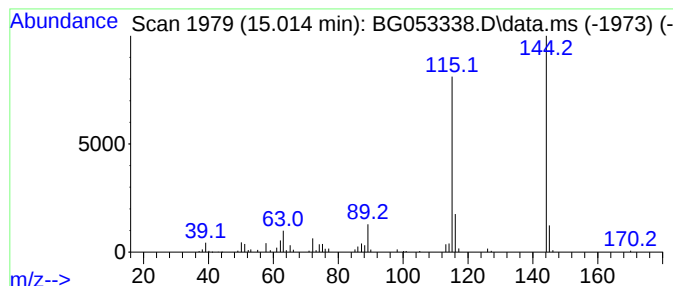
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Naphthalenol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.014	13.15 ng	165023	Acenaphthene-d10	14.726

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Naphthalenol	144	C10H8O	000135-19-3	97
2		Furan, 3-phenyl-	144	C10H8O	013679-41-9	91
3		Benzofuran, 2-ethenyl-	144	C10H8O	007522-79-4	91
4		1-Naphthalenol	144	C10H8O	000090-15-3	91
5		Carbaril	201	C12H11NO2	000063-25-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053338.D
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Operator : CG/JU
Sample : N2482-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

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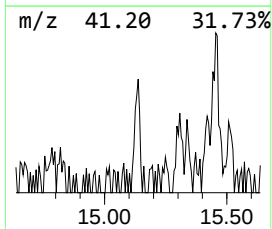
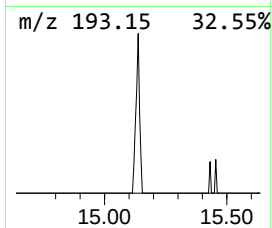
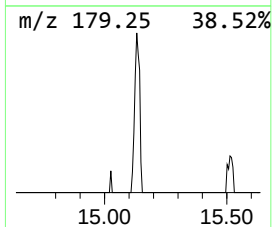
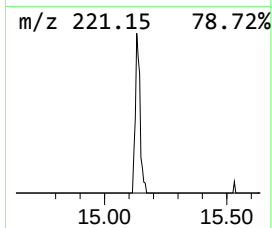
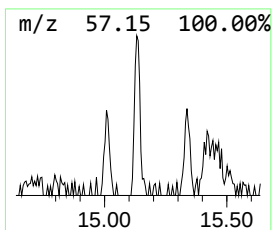
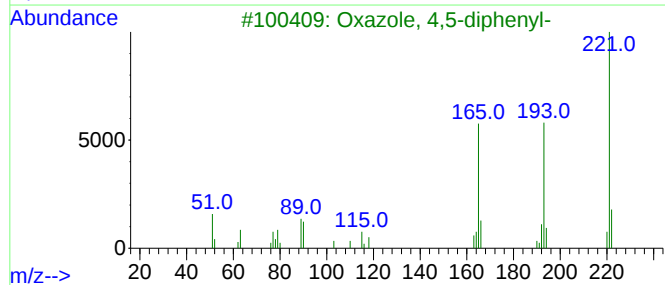
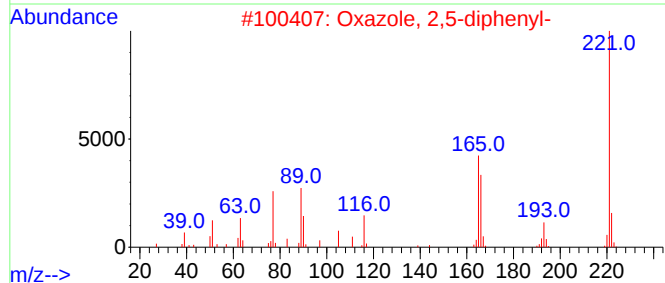
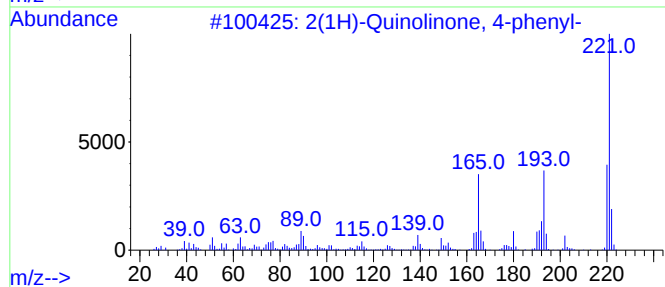
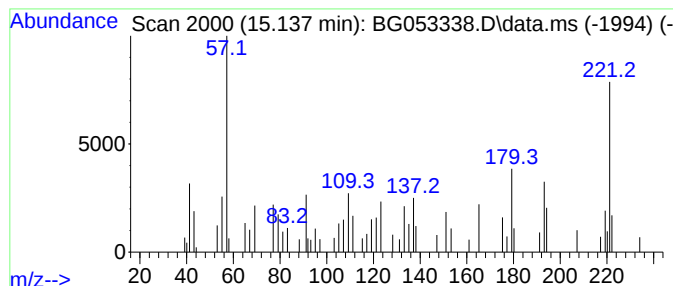
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.137 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.137	2.80 ng	35108	Acenaphthene-d10	14.726

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Quinolinone, 4-phenyl-			221	C15H11NO	005855-57-2	43
2	Oxazole, 2,5-diphenyl-			221	C15H11NO	000092-71-7	43
3	Oxazole, 4,5-diphenyl-			221	C15H11NO	004675-18-7	43
4	6-Methyladenine, TMS derivative			221	C9H15N5Si	032865-83-1	38
5	1H-1,2,3-Triazole, 4,5-diphenyl-			221	C14H11N3	005533-73-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053338.D
Acq On : 27 Apr 2022 2:39
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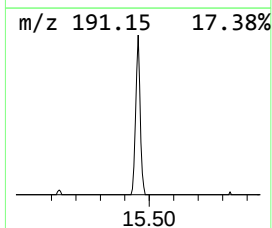
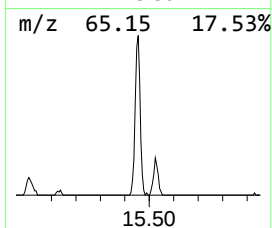
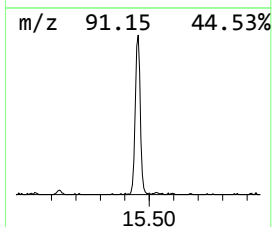
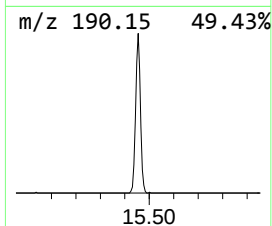
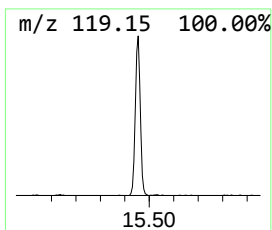
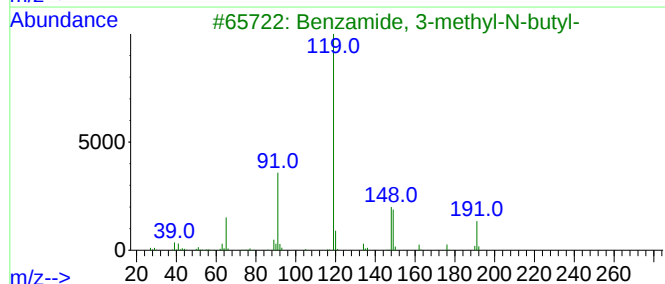
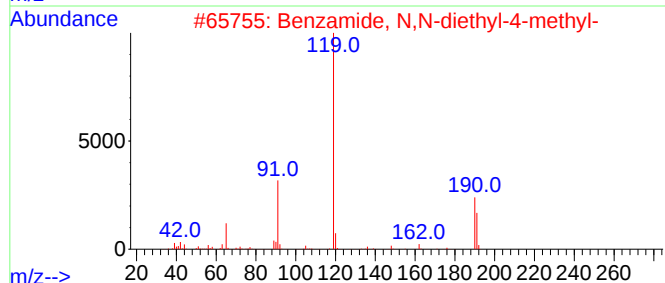
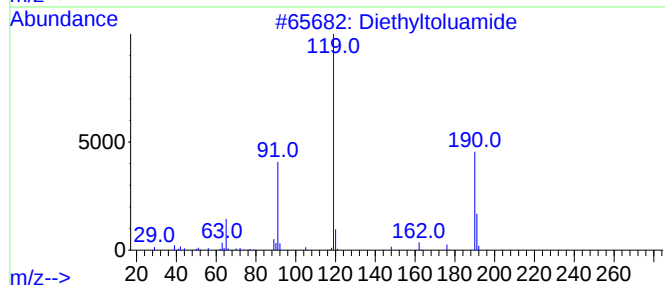
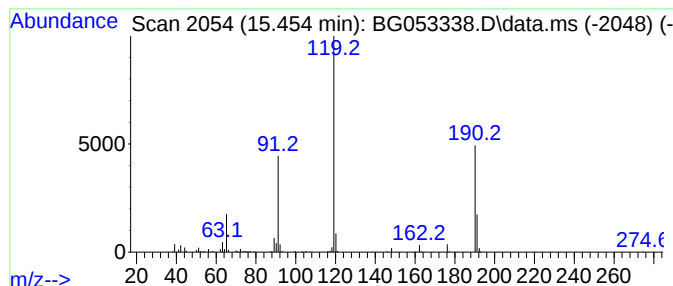
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Diethyltoluamide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.454	21.77 ng	273210	Acenaphthene-d10	14.726

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyltoluamide	191	C12H17NO	000134-62-3	96
2			Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	87
3			Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	76
4			Benzamide, 4-methyl-N-butyl-	191	C12H17NO	1000407-46-6	68
5			1-Propanone, 2-methyl-1-(2-methy...	162	C11H14O	002040-21-3	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053338.D
Acq On : 27 Apr 2022 2:39
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EB-2022-04-19

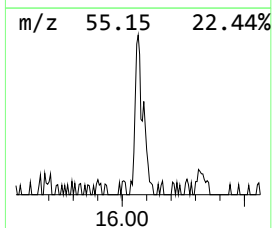
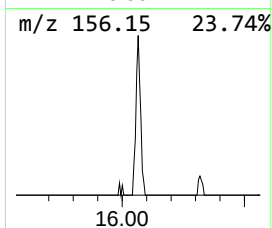
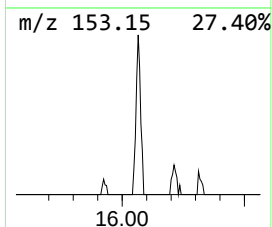
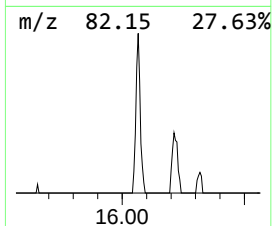
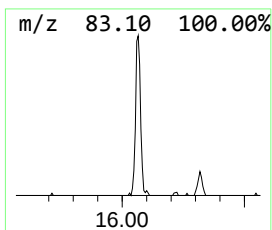
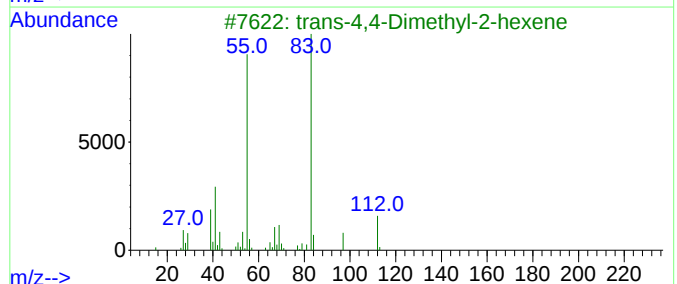
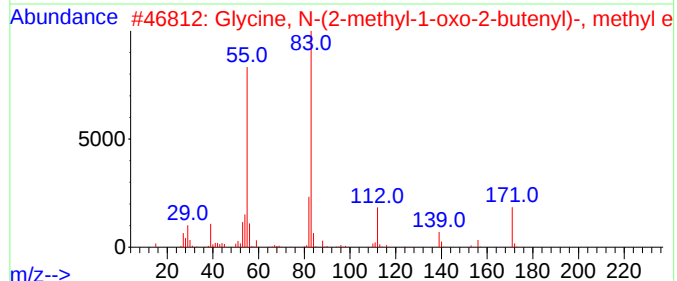
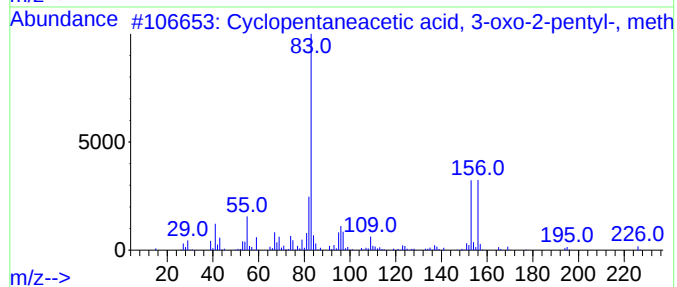
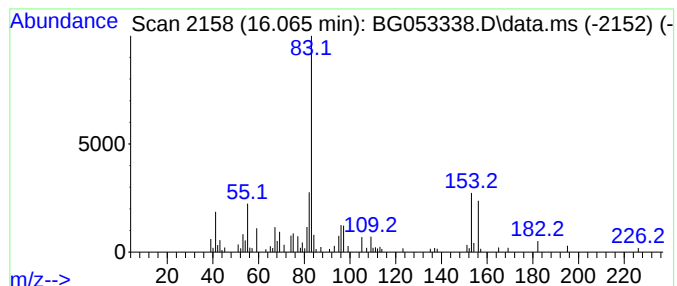
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclopentaneacetic acid, 3-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.065	6.98 ng	87524	Acenaphthene-d10	14.726

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	95
2			Glycine, N-(2-methyl-1-oxo-2-but...	171	C8H13NO3	055649-53-1	43
3			trans-4,4-Dimethyl-2-hexene	112	C8H16	019550-83-5	38
4			Heptylcyclohexane	182	C13H26	005617-41-4	38
5			2-Butenoic acid, 3-methyl-, meth...	114	C6H10O2	000924-50-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
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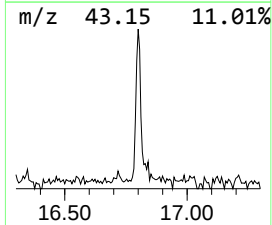
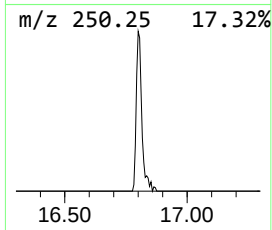
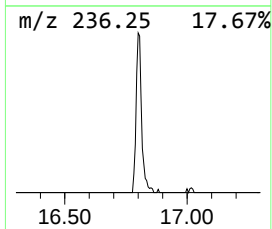
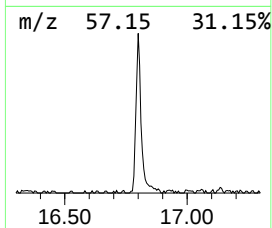
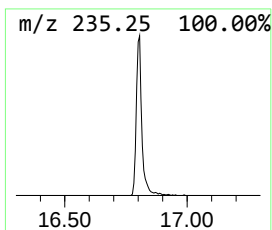
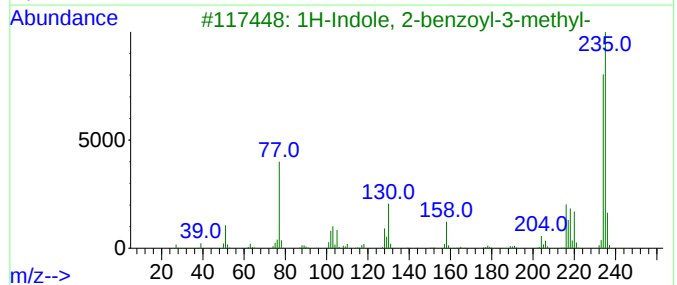
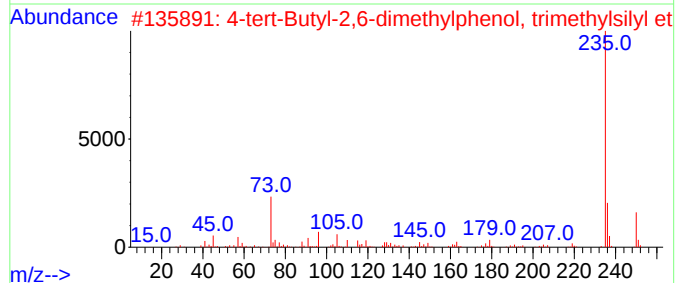
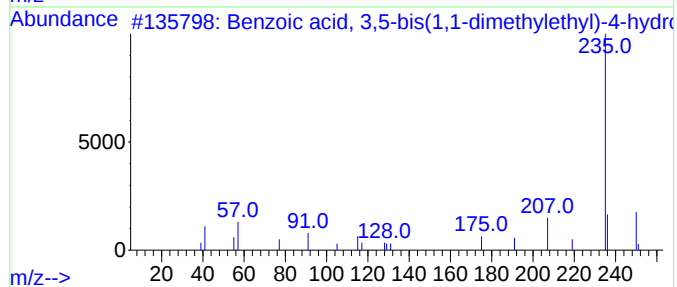
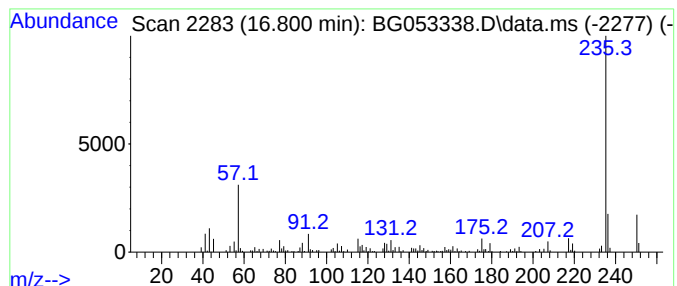
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzoic acid, 3,5-bis(1,1-d... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.800	14.86 ng	284537	Phenanthrene-d10	17.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 3,5-bis(1,1-dimeth...	250	C15H22O3	001421-49-4	90
2			4-tert-Butyl-2,6-dimethylphenol,...	250	C15H26OSi	1000495-37-2	87
3			1H-Indole, 2-benzoyl-3-methyl-	235	C16H13NO	001025-97-4	72
4			4-[Acetyloxy-(2-pyridyl)methyl]-...	294	C17H14N2O3	093323-89-8	64
5			Imidazo[1',2'-a]pyrido[3,2-c]qui...	235	C14H9N3O	129011-77-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053338.D
Acq On : 27 Apr 2022 2:39
Operator : CG/JU
Sample : N2482-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-2022-04-19

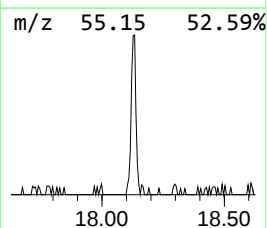
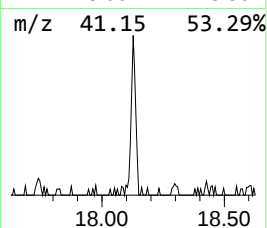
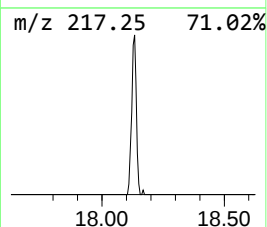
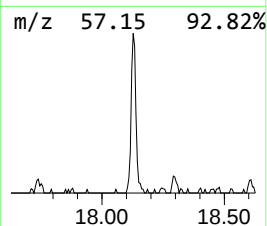
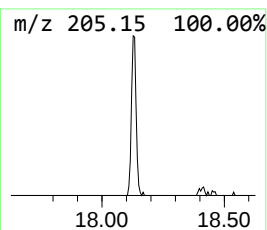
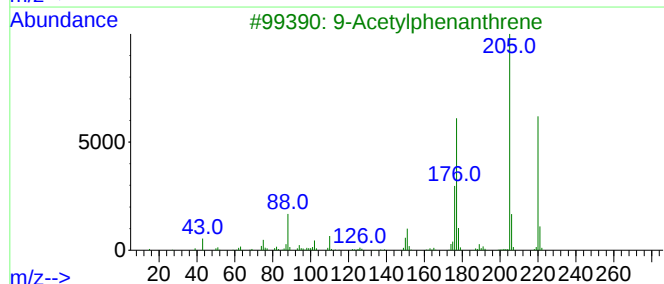
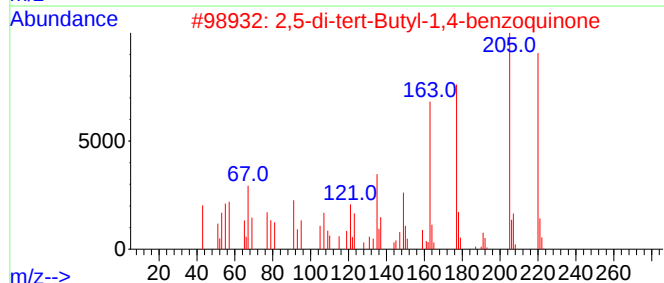
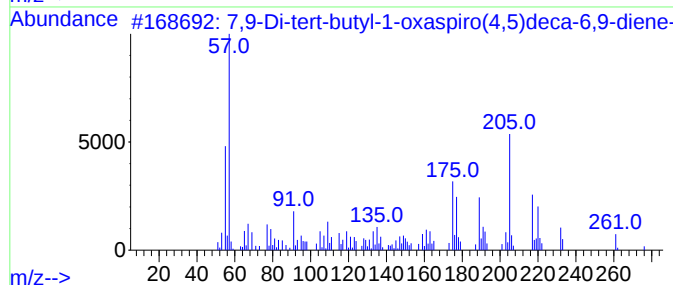
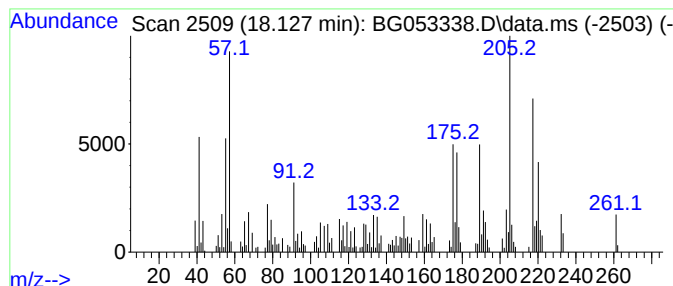
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	7.93 ng	151897	Phenanthrene-d10	17.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	87		
2	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	51		
3	9-Acetylphenanthrene	220	C16H12O	002039-77-2	45		
4	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45		
5	Ethanone, 1-(9-anthracenyl)-	220	C16H12O	000784-04-3	45		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053338.D
Acq On : 27 Apr 2022 2:39
Operator : CG/JU
Sample : N2482-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB-2022-04-19

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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
Oxalic acid, is...	8.158	4.3	ng	24810	1	8.105	114867	20.0
Ethanol, 2-(hex...	9.427	7.0	ng	40141	1	8.105	114867	20.0
Ethanol, 1-(2-b...	10.679	4.5	ng	36073	2	10.913	161860	20.0
Ethanol, 2-phen...	11.272	3.4	ng	27810	2	10.913	161860	20.0
3-Heptyl isobut...	13.087	7.2	ng	90135	3	14.726	250961	20.0
Phenol, 4-(1,1-...	13.569	63.5	ng	796987	3	14.726	250961	20.0
Vanillin	13.645	6.0	ng	75542	3	14.726	250961	20.0
2-Naphthalenol	15.014	13.2	ng	165023	3	14.726	250961	20.0
unknown15.137	15.137	2.8	ng	35108	3	14.726	250961	20.0
Diethyltoluamide	15.454	21.8	ng	273210	3	14.726	250961	20.0
Cyclopentaneace...	16.065	7.0	ng	87524	3	14.726	250961	20.0
Benzoic acid, 3...	16.800	14.9	ng	284537	4	17.475	382969	20.0
7,9-Di-tert-but...	18.127	7.9	ng	151897	4	17.475	382969	20.0