

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101122\
 Data File : BG055132.D
 Acq On : 11 Oct 2022 18:41
 Operator : CG/JU
 Sample : N5082-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FLORENCE-COMP-1-FLORENCE-VOC-1

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-BG100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055132.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.364	8	13	30	rVB	262115	394466	20.79%	3.027%
2	5.373	348	355	362	rBV	116022	178352	9.40%	1.369%
3	5.849	428	436	449	rVB	514716	828346	43.65%	6.356%
4	7.459	701	710	723	rBV	551376	950579	50.09%	7.294%
5	8.329	850	858	871	rBV	128749	216227	11.39%	1.659%
6	9.498	1049	1057	1067	rBV	322753	581617	30.65%	4.463%
7	10.902	1290	1296	1302	rBV2	24469	38871	2.05%	0.298%
8	11.161	1332	1340	1348	rBV	190329	340296	17.93%	2.611%
9	13.564	1742	1749	1756	rBV	891255	1362265	71.78%	10.453%
10	14.768	1946	1954	1958	rBV2	25590	38573	2.03%	0.296%
11	14.892	1966	1975	1979	rBV	454804	687000	36.20%	5.272%
12	14.939	1979	1983	1989	rVB	309585	475982	25.08%	3.652%
13	15.174	2017	2023	2028	rBV	43803	61933	3.26%	0.475%
14	16.302	2210	2215	2220	rBV2	15314	22595	1.19%	0.173%
15	16.413	2220	2234	2241	rBV	714243	1161061	61.18%	8.909%
16	17.671	2441	2448	2453	rBV	387191	601043	31.67%	4.612%
17	18.523	2589	2593	2597	rBV5	21514	37547	1.98%	0.288%
18	19.698	2789	2793	2797	rVB	43274	64459	3.40%	0.495%
19	20.062	2851	2855	2860	rVB	33142	52096	2.75%	0.400%
20	20.244	2880	2886	2892	rVB	1324212	1702621	89.72%	13.065%
21	21.384	3074	3080	3087	rVB	1378589	1897782	100.00%	14.563%
22	21.560	3105	3110	3116	rBV2	82032	129200	6.81%	0.991%
23	21.960	3172	3178	3184	rBV	331582	588019	30.98%	4.512%
24	25.403	3756	3764	3775	rVB2	207172	620968	32.72%	4.765%

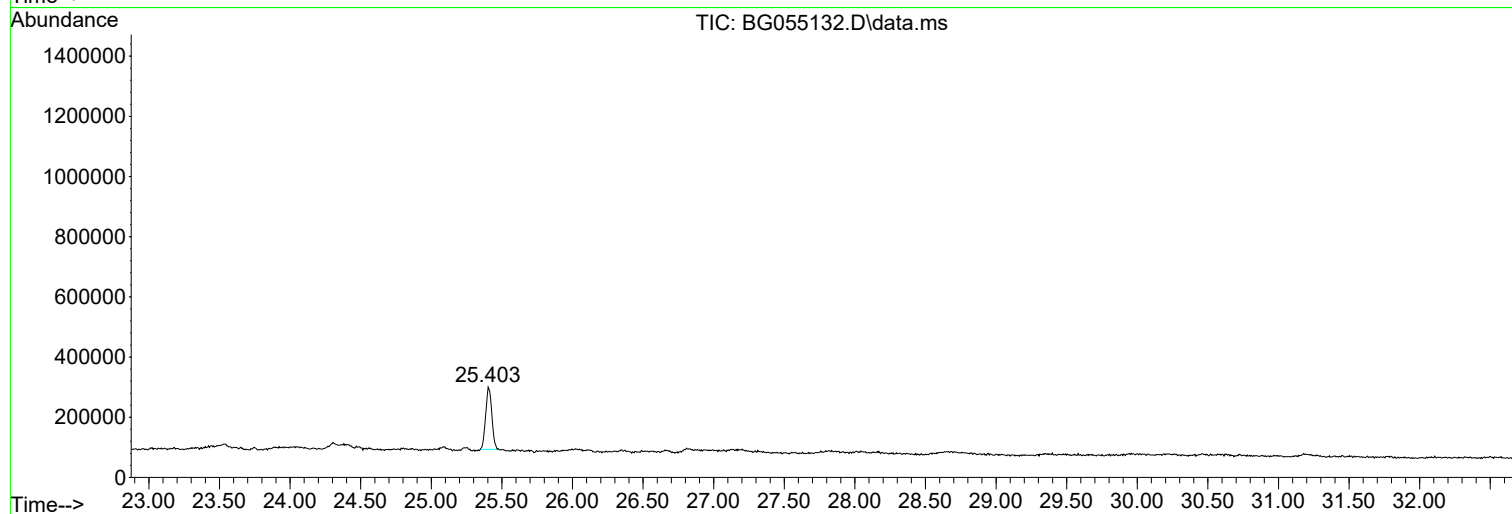
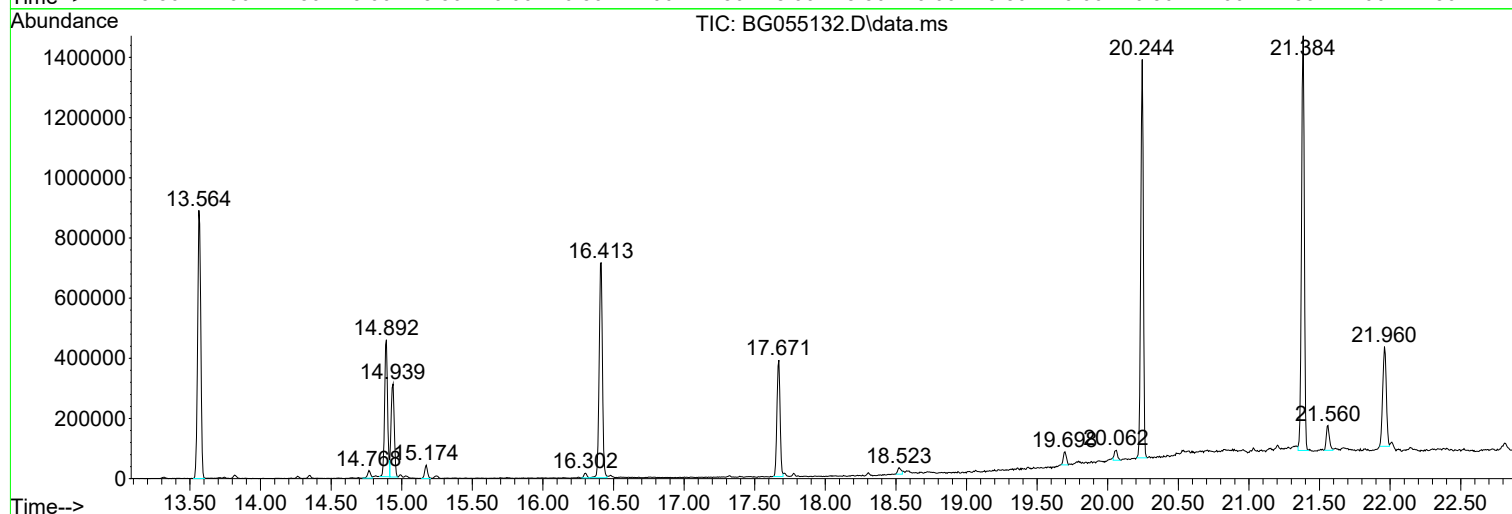
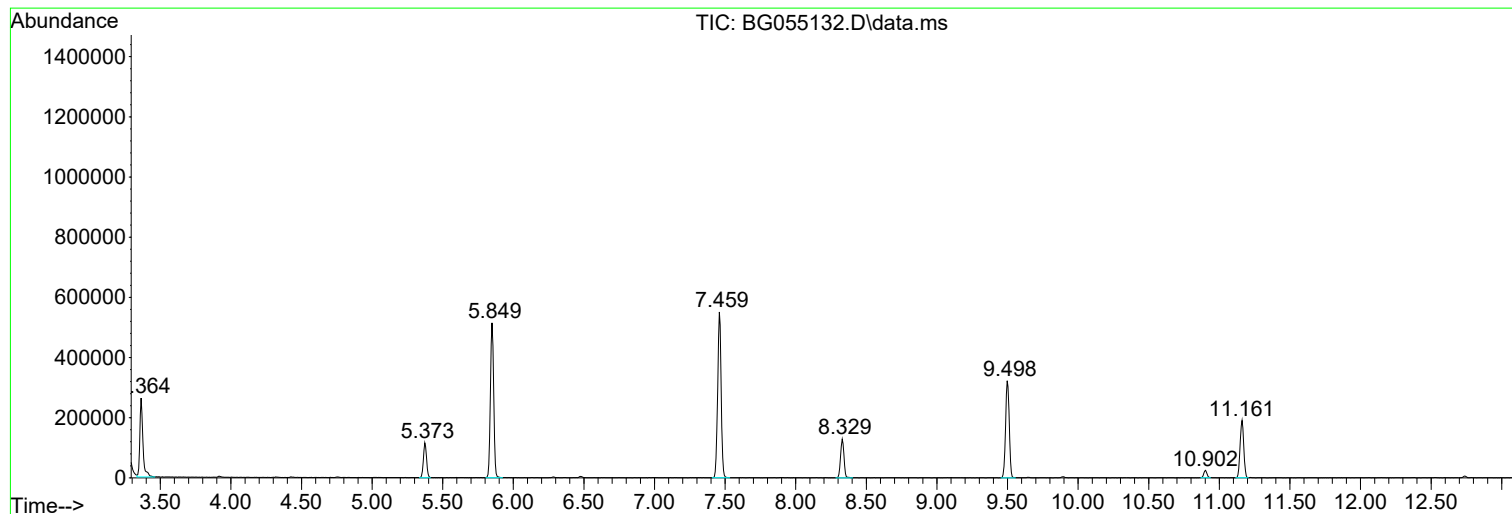
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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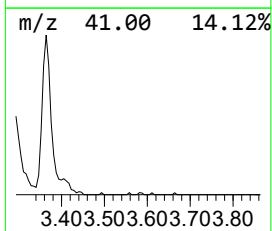
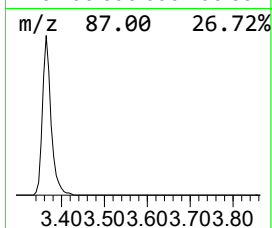
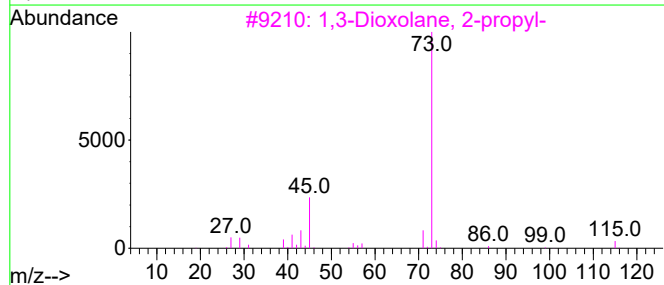
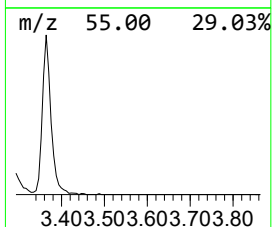
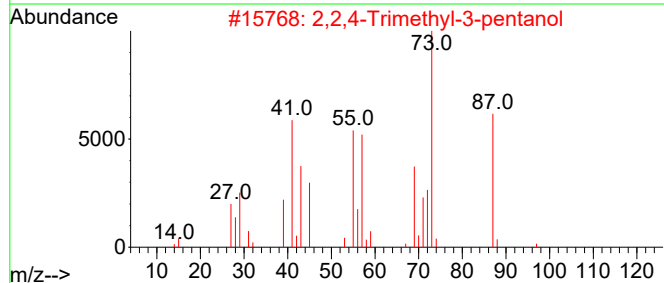
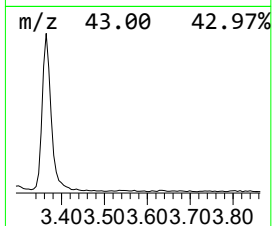
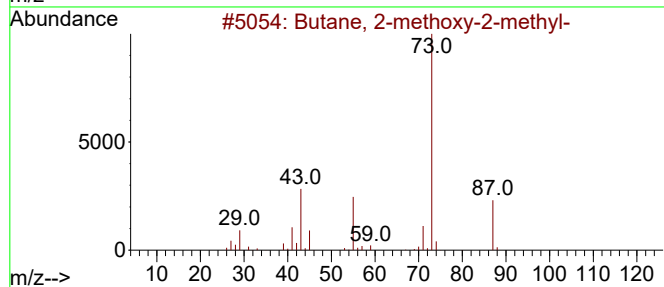
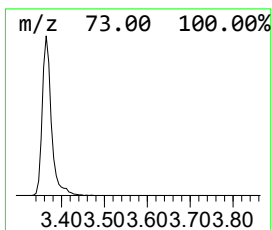
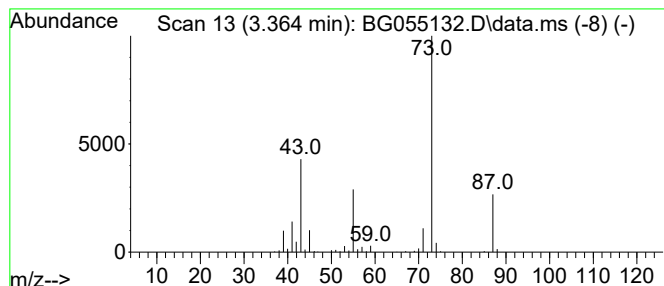
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	36.49 ng	394466	1,4-Dichlorobenzene-d4	8.329

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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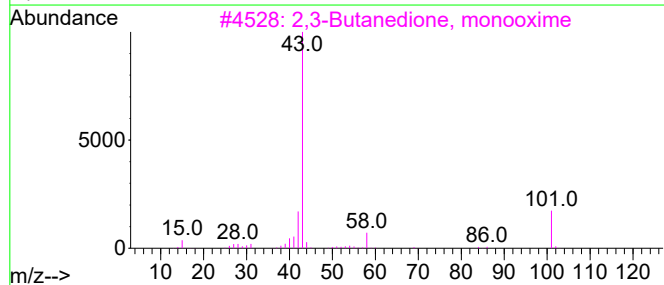
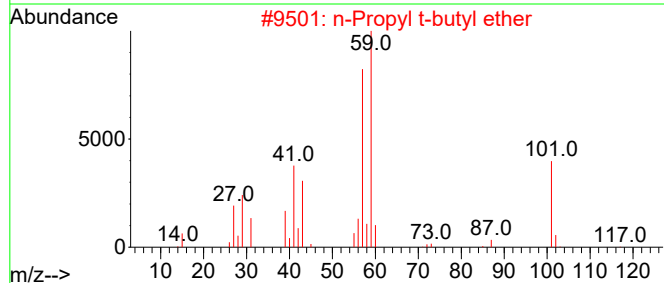
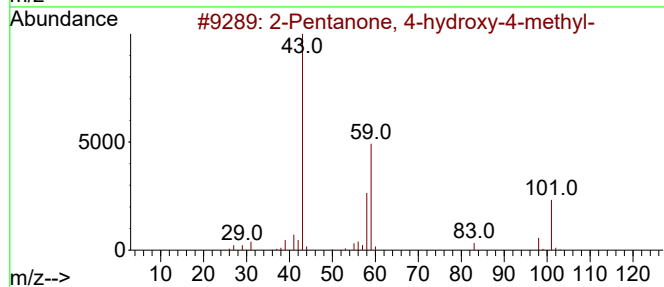
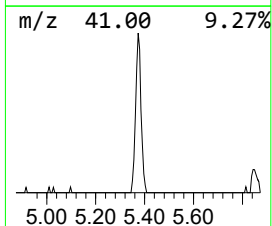
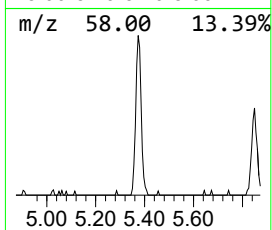
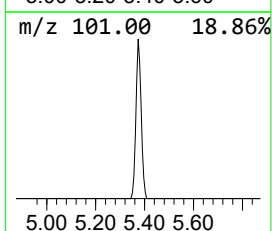
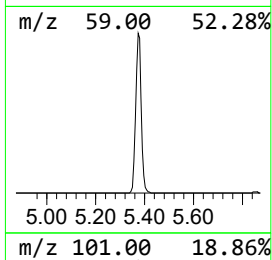
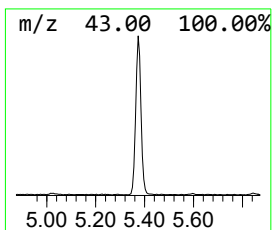
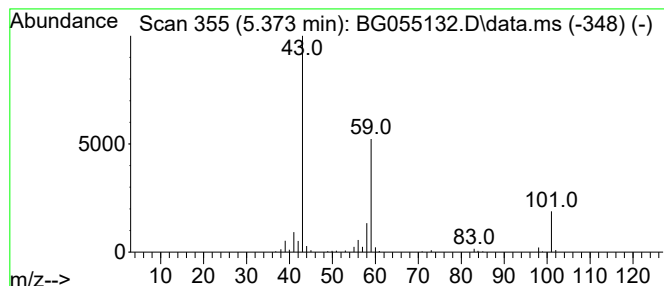
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.373	16.50 ng	178352	1,4-Dichlorobenzene-d4	8.329

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1,2-Butanediol	90	C4H10O2	000584-03-2	23



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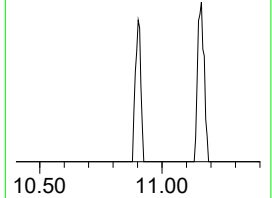
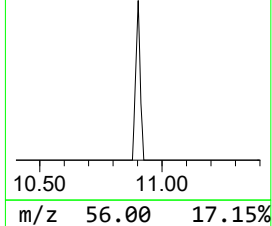
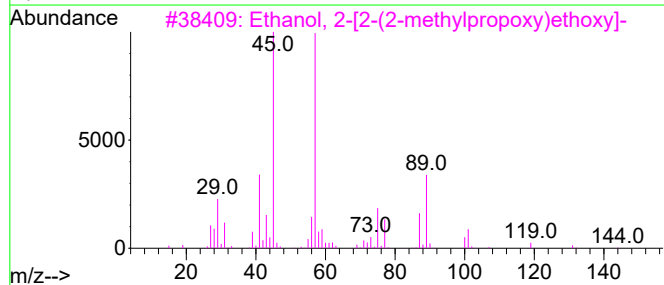
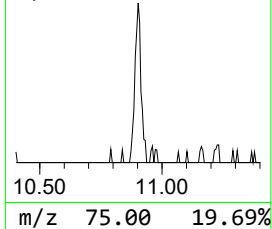
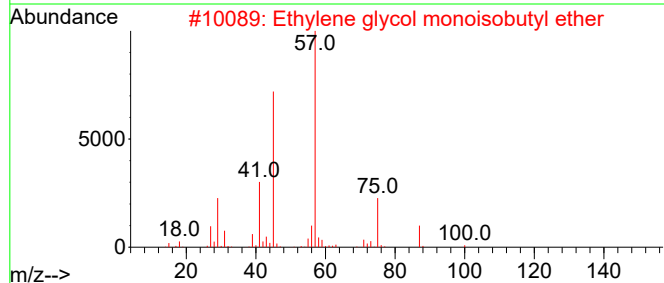
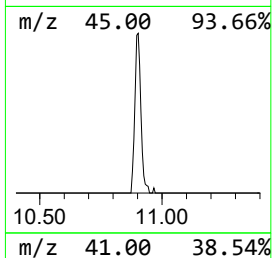
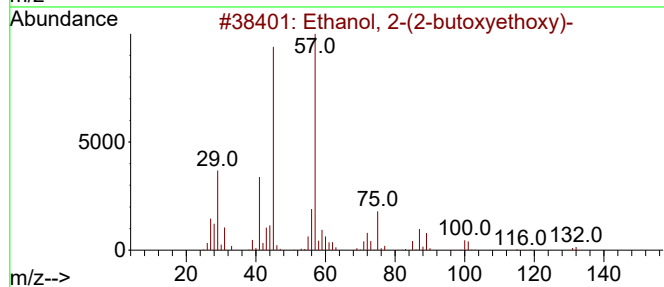
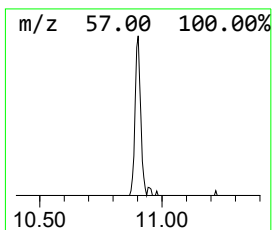
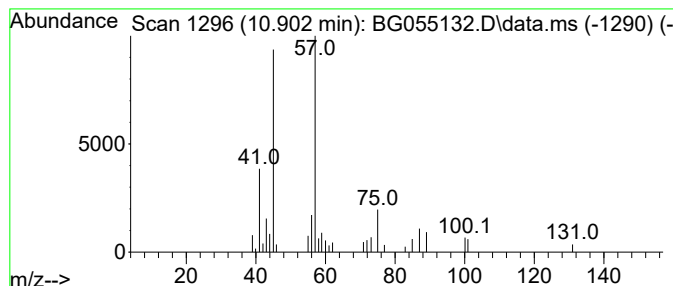
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.902	2.28 ng	38871	Naphthalene-d8	11.161

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	50
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5			Ethanol, 2-[2-(2-butoxyethoxy)ethoxy]-	206	C10H22O4	000143-22-6	45



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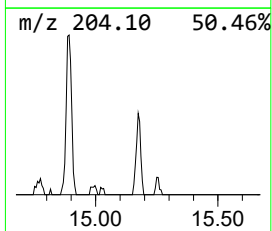
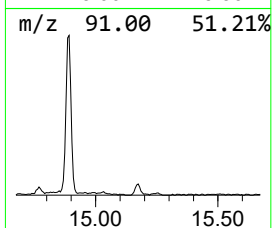
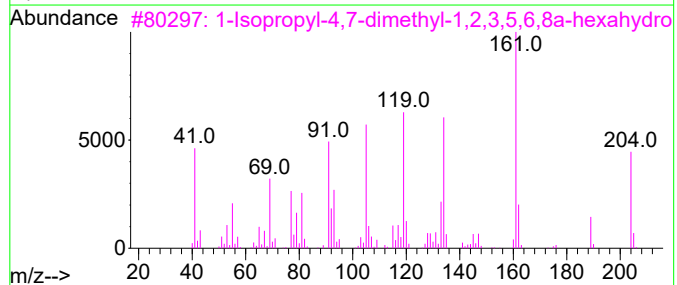
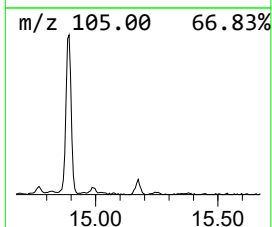
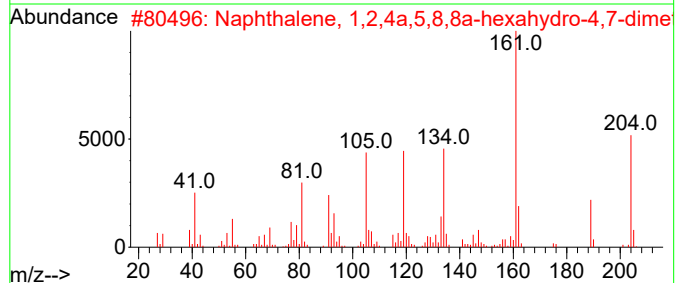
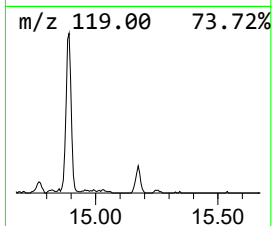
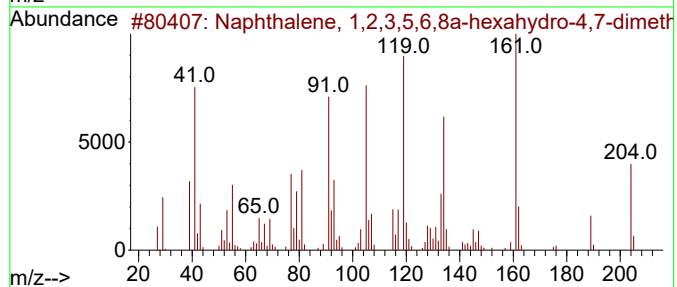
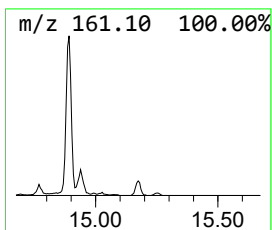
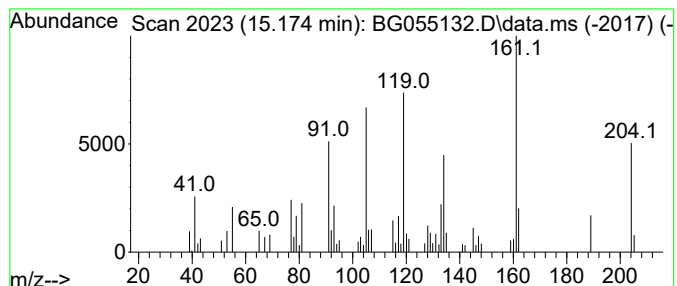
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Peak Number 4 Naphthalene, 1,2,3,5,6,8a-h... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	2.60 ng	61933	Acenaphthene-d10	14.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	98
2			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	94
3			1-Isopropyl-4,7-dimethyl-1,2,3,5...	204	C15H24	016729-01-4	87
4			isolekene	204	C15H24	095910-36-4	81
5			.alpha.-Cubebene	204	C15H24	017699-14-8	70



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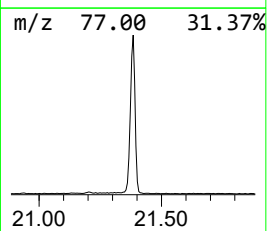
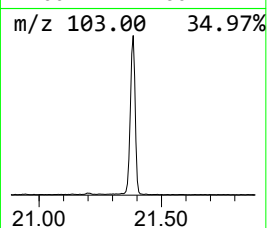
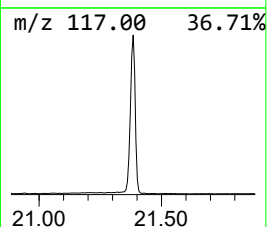
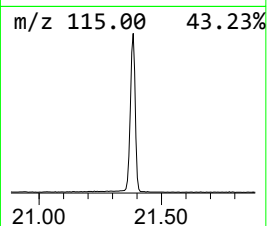
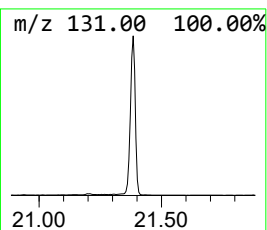
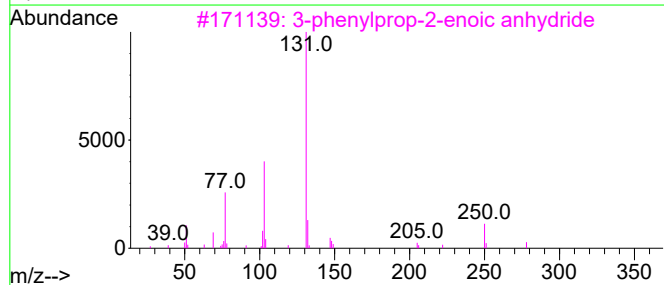
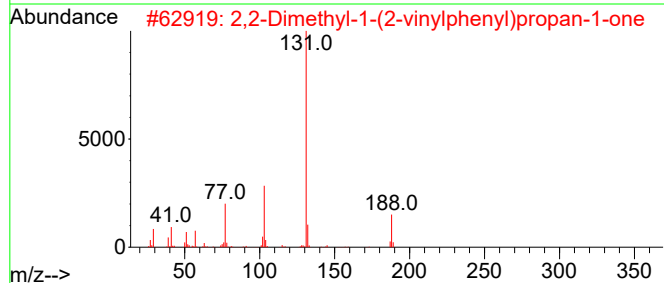
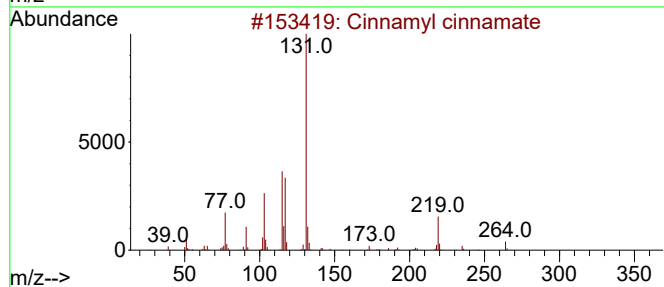
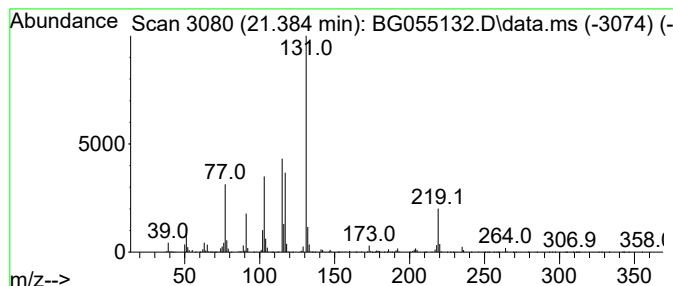
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.384	64.55 ng	1897780	Chrysene-d12	21.960

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	60
3			3-phenylprop-2-enoic anhydride	278	C18H14O3	1010401-87-5	47
4			(2E)-N-(4-Methylphenyl)-3-phenyl...	237	C16H15NO	134430-88-9	47
5			Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	47



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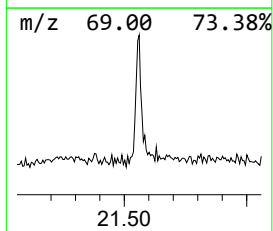
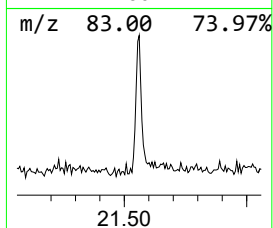
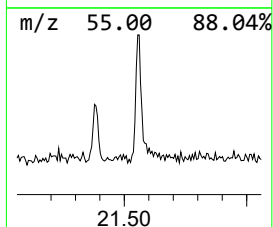
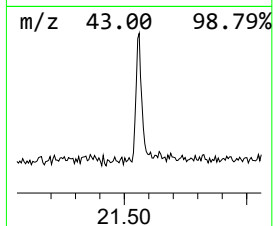
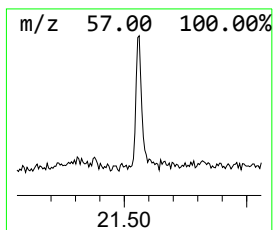
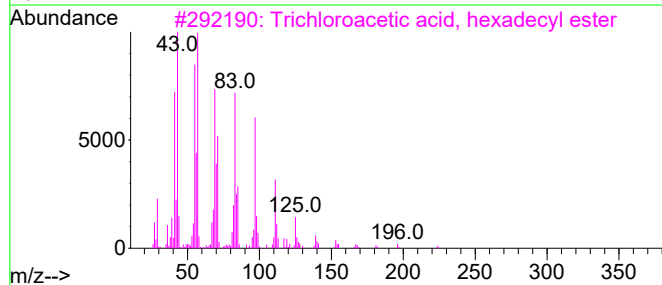
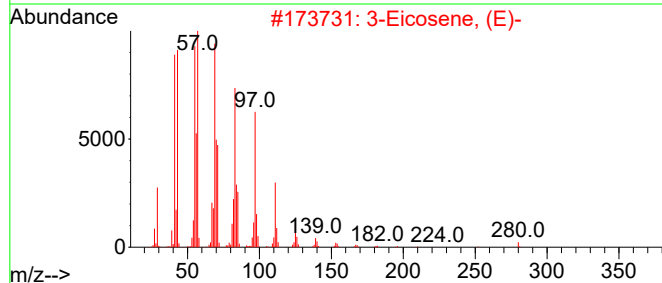
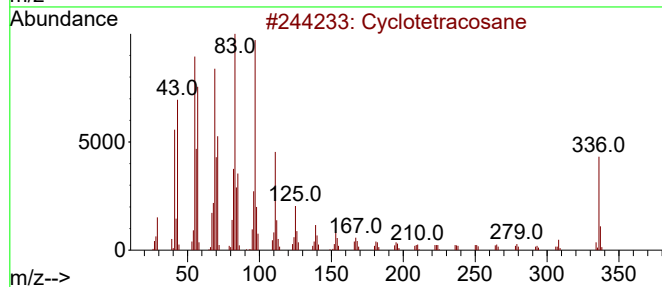
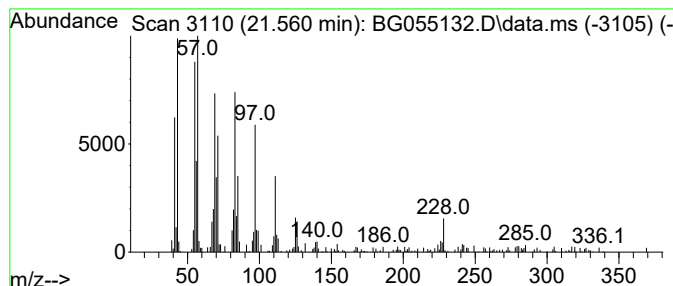
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.560	4.39 ng	129200	Chrysene-d12	21.960

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	93
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			9-Eicosene, (E)-	280	C20H40	074685-29-3	90
5			1-Hexacosene	364	C26H52	018835-33-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101122\
Data File : BG055132.D
Acq On : 11 Oct 2022 18:41
Operator : CG/JU
Sample : N5082-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FLORENCE-COMP-1-FLORENCE-VOC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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
Butane, 2-metho...	3.364	36.5	ng	394466	1	8.329	216227	20.0
2-Pentanone, 4-...	5.373	16.5	ng	178352	1	8.329	216227	20.0
Ethanol, 2-(2-b...	10.902	2.3	ng	38871	2	11.161	340296	20.0
Naphthalene, 1,...	15.174	2.6	ng	61933	3	14.939	475982	20.0
Cinnamyl cinnamate	21.384	64.5	ng	1897780	5	21.960	588019	20.0
Cyclotetracosane	21.560	4.4	ng	129200	5	21.960	588019	20.0