

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
 Data File : BG056542.D
 Acq On : 3 Feb 2023 17:11
 Operator : CG/JU
 Sample : 01348-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 W-H5(31-32)

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-BG012723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.036	114	127	132	rBV3	40581	158320	3.66%	0.321%
2	4.101	132	138	148	rVV3	45301	171793	3.97%	0.349%
3	4.212	154	157	170	rVB7	31174	95306	2.20%	0.193%
4	5.311	336	344	352	rVB	106064	185601	4.29%	0.377%
5	5.799	421	427	434	rVB	420368	690552	15.97%	1.401%
6	6.233	492	501	532	rBV	919155	4325231	100.00%	8.775%
7	7.426	696	704	711	rVV	430418	768785	17.77%	1.560%
8	7.931	782	790	799	rBV	1172226	3509939	81.15%	7.121%
9	8.014	799	804	833	rVB	612228	2179427	50.39%	4.421%
10	8.272	844	848	860	rVB	124334	234107	5.41%	0.475%
11	8.560	892	897	909	rBV4	45872	119300	2.76%	0.242%
12	8.825	935	942	954	rBV	454773	1425797	32.96%	2.893%
13	9.383	1034	1037	1042	rVB2	66564	94358	2.18%	0.191%
14	9.453	1043	1049	1053	rVV	232445	422589	9.77%	0.857%
15	9.488	1053	1055	1060	rVB2	84914	118533	2.74%	0.240%
16	9.553	1060	1066	1077	rBV2	199184	570407	13.19%	1.157%
17	9.665	1081	1085	1092	rVB	78778	145978	3.38%	0.296%
18	9.976	1134	1138	1146	rVB6	55648	111153	2.57%	0.225%
19	10.058	1147	1152	1157	rBV	117691	219213	5.07%	0.445%
20	10.135	1157	1165	1171	rBV3	215591	651379	15.06%	1.321%
21	10.528	1227	1232	1238	rVB4	101299	218236	5.05%	0.443%
22	10.599	1240	1244	1248	rBV3	57451	88830	2.05%	0.180%
23	10.769	1267	1273	1275	rBV	96870	191844	4.44%	0.389%
24	10.916	1295	1298	1304	rVB6	59786	98932	2.29%	0.201%
25	11.040	1316	1319	1325	rVB	99178	145213	3.36%	0.295%
26	11.110	1326	1331	1334	rVV	137368	259260	5.99%	0.526%
27	11.157	1334	1339	1345	rVB	338864	652016	15.07%	1.323%
28	11.316	1361	1366	1372	rVB2	176708	322559	7.46%	0.654%
29	11.615	1411	1417	1424	rBV2	194192	553199	12.79%	1.122%
30	11.756	1435	1441	1456	rVB	200509	636708	14.72%	1.292%
31	12.743	1604	1609	1618	rBV2	231385	443854	10.26%	0.900%
32	12.937	1637	1642	1643	rBV	154486	217171	5.02%	0.441%
33	13.519	1736	1741	1753	rVB	963089	1592701	36.82%	3.231%
34	13.889	1797	1804	1815	rBV2	416248	1016764	23.51%	2.063%
35	14.148	1843	1848	1856	rBV	544028	992753	22.95%	2.014%
36	14.218	1857	1860	1866	rVB2	92411	150026	3.47%	0.304%

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Integrator: RTE

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Stop Thrs : 0

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.312	1872	1876	1878	rBV	156375	255909	5.92%	0.519%
38	14.606	1920	1926	1931	rBV	1304970	2024958	46.82%	4.108%
39	14.759	1947	1952	1956	rBV2	413883	669358	15.48%	1.358%
40	14.841	1961	1966	1970	rBV2	226562	428443	9.91%	0.869%
41	14.923	1972	1980	1989	rVB4	758736	1754269	40.56%	3.559%
42	15.135	2012	2016	2021	rBV	239036	348001	8.05%	0.706%
43	15.188	2021	2025	2030	rVV4	202548	368624	8.52%	0.748%
44	15.246	2030	2035	2039	rVV	585896	865049	20.00%	1.755%
45	15.299	2040	2044	2048	rVB2	228080	338140	7.82%	0.686%
46	15.370	2049	2056	2063	rBV6	286214	623970	14.43%	1.266%
47	15.534	2080	2084	2088	rBV3	218575	296278	6.85%	0.601%
48	15.587	2089	2093	2097	rBV3	221439	337260	7.80%	0.684%
49	15.664	2103	2106	2109	rBV3	97183	143435	3.32%	0.291%
50	15.711	2110	2114	2122	rVB4	379341	847305	19.59%	1.719%
51	16.222	2198	2201	2209	rBV4	163865	287628	6.65%	0.584%
52	16.386	2224	2229	2236	rVB	595615	1001440	23.15%	2.032%
53	16.557	2253	2258	2265	rBV6	565968	1307289	30.22%	2.652%
54	16.721	2282	2286	2292	rVB	660081	917953	21.22%	1.862%
55	16.821	2300	2303	2314	rVB9	221886	470780	10.88%	0.955%
56	16.927	2317	2321	2337	rVB3	435750	1116313	25.81%	2.265%
57	17.291	2377	2383	2390	rBV2	961273	2258473	52.22%	4.582%
58	17.391	2397	2400	2408	rVB3	553500	889455	20.56%	1.804%
59	17.497	2414	2418	2427	rVB	655392	1388808	32.11%	2.818%
60	17.638	2439	2442	2448	rVB	286822	403337	9.33%	0.818%
61	17.832	2471	2475	2478	rBV	384258	565117	13.07%	1.146%
62	18.031	2507	2509	2514	rVB	438331	555738	12.85%	1.127%
63	18.143	2525	2528	2537	rVB4	401966	745719	17.24%	1.513%
64	18.319	2555	2558	2562	rVB	317796	386903	8.95%	0.785%
65	19.465	2749	2753	2759	rVB	973458	1298322	30.02%	2.634%
66	19.547	2765	2767	2772	rVB	444176	550329	12.72%	1.116%
67	20.217	2877	2881	2889	rVB	1639863	2069379	47.84%	4.198%

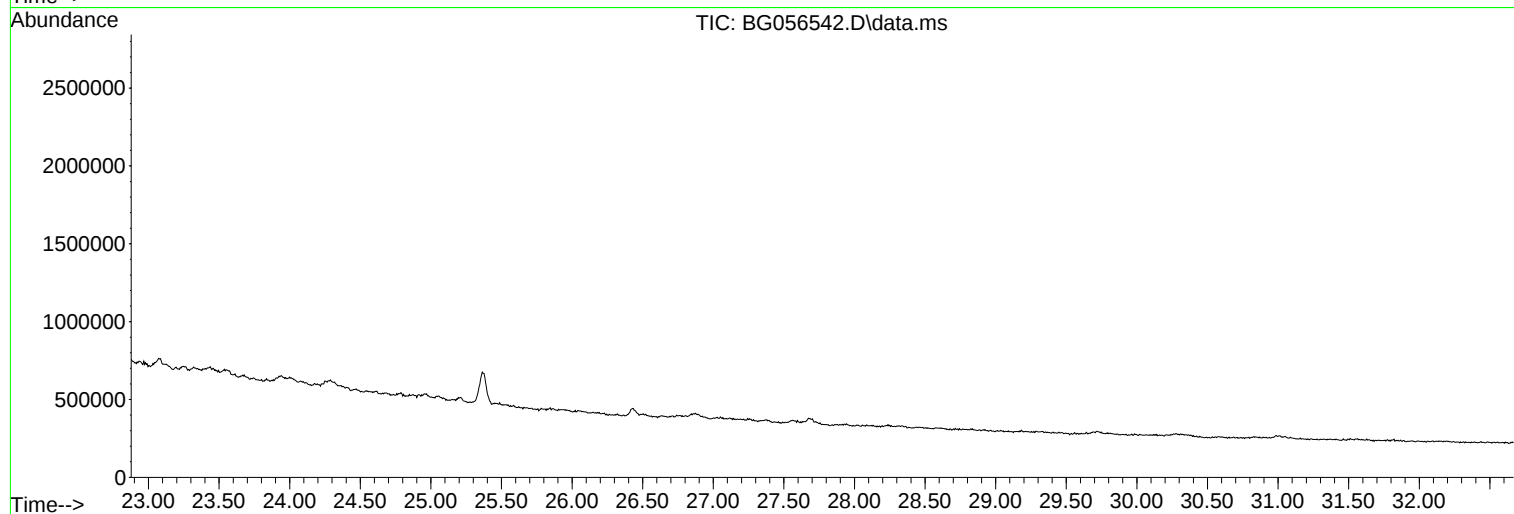
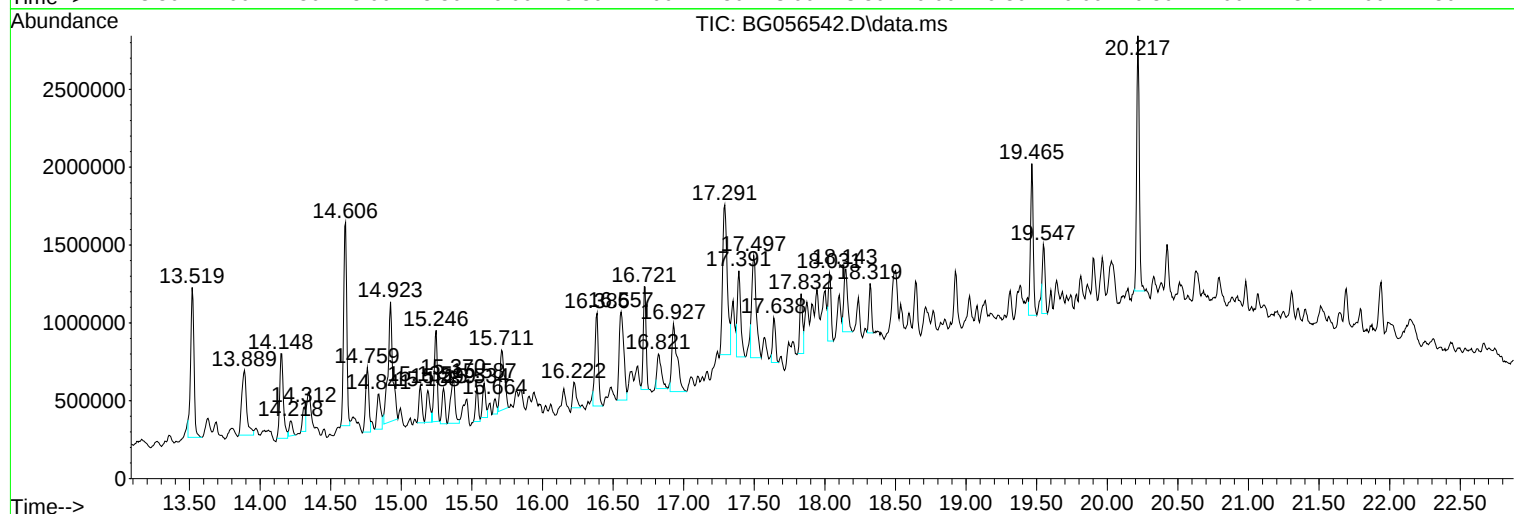
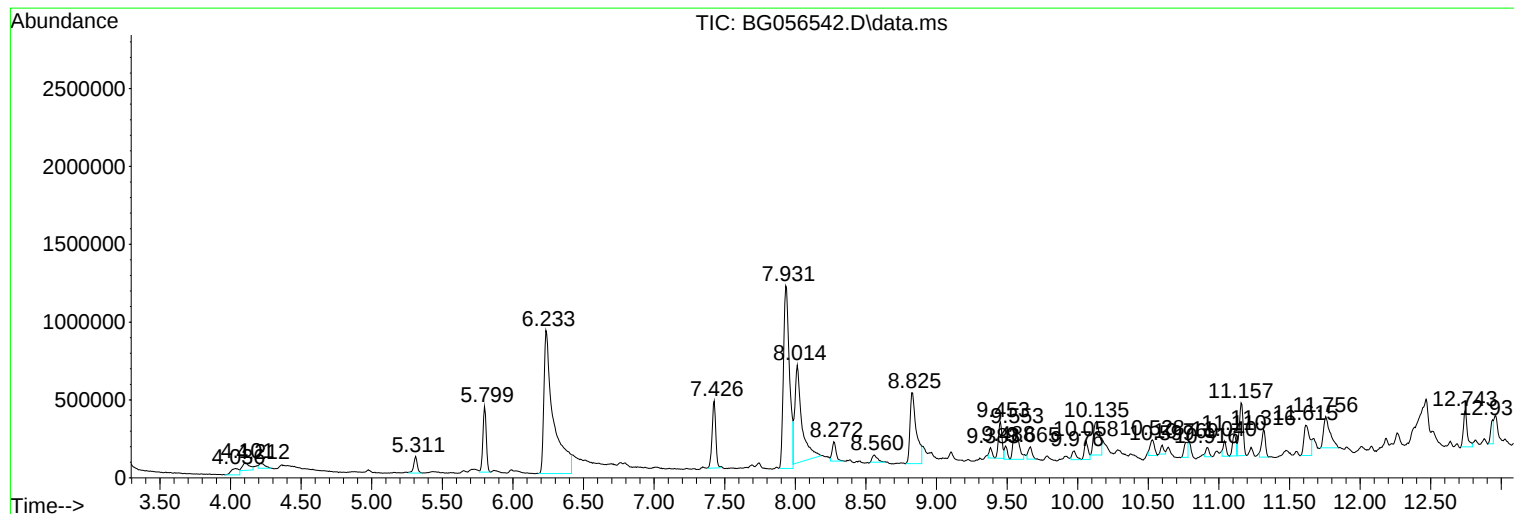
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Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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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Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

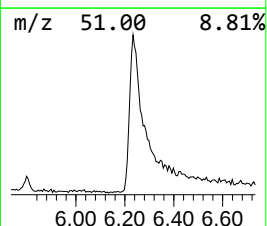
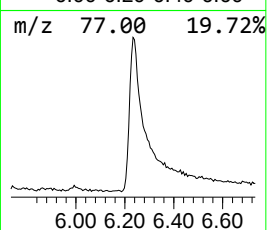
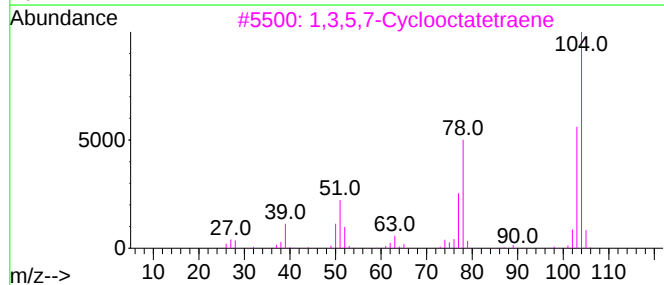
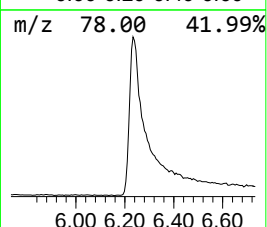
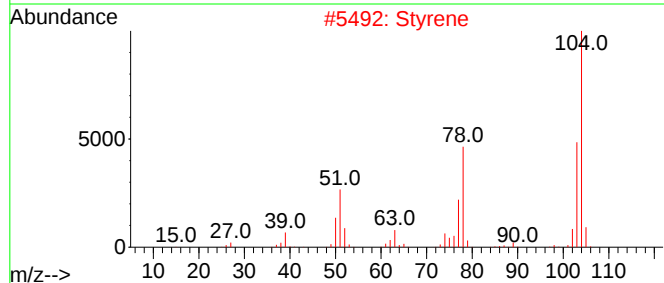
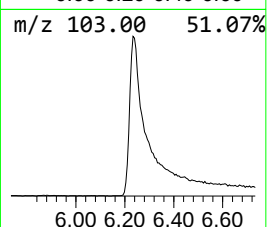
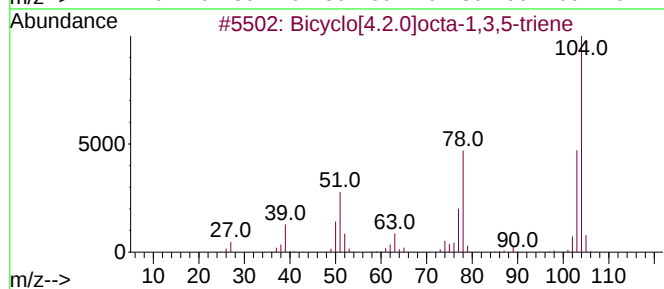
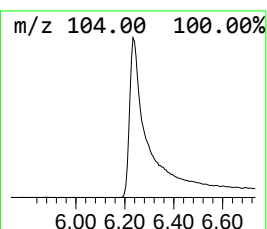
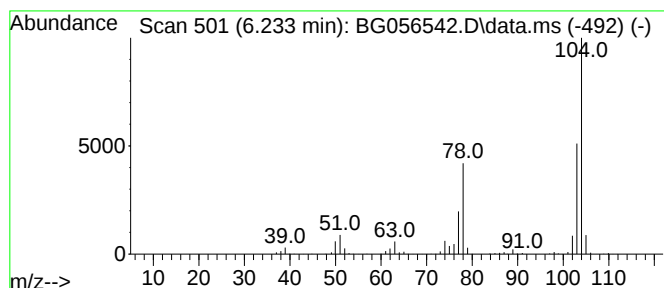
Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.233	369.51 ng	4325230	1,4-Dichlorobenzene-d4	8.272	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	95
2	Styrene	104	C8H8	000100-42-5	95
3	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	91
4	2-Methylbenzyl alcohol, trifluor...	218	C10H9F3O2	1000364-57-0	28
5	Acetic acid, 2-phenylethyl ester	164	C10H12O2	000103-45-7	23



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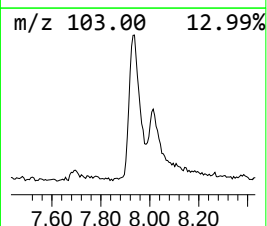
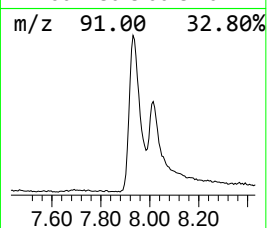
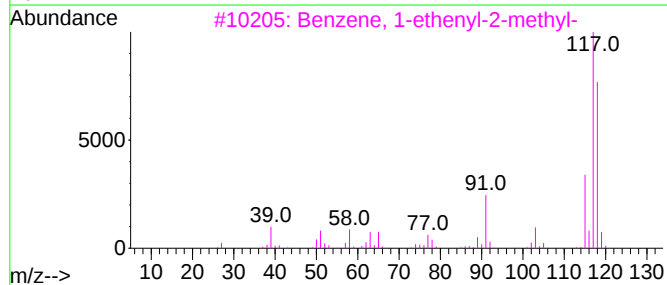
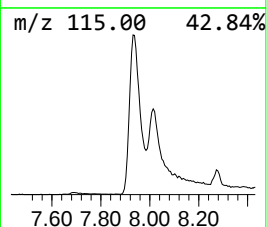
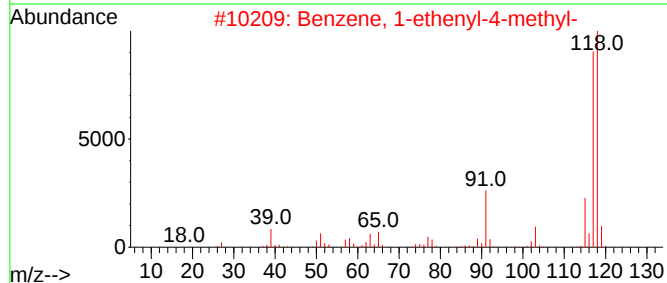
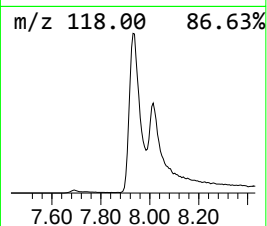
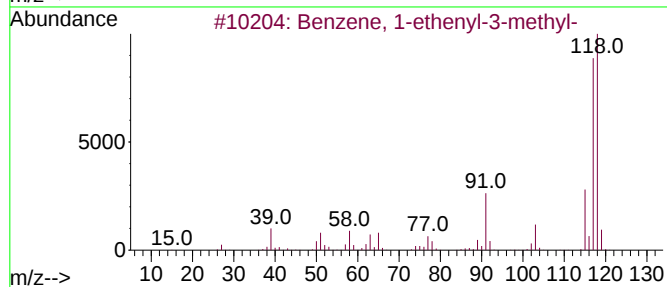
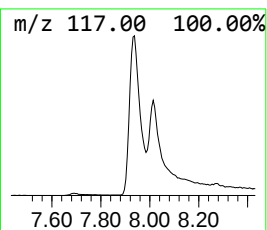
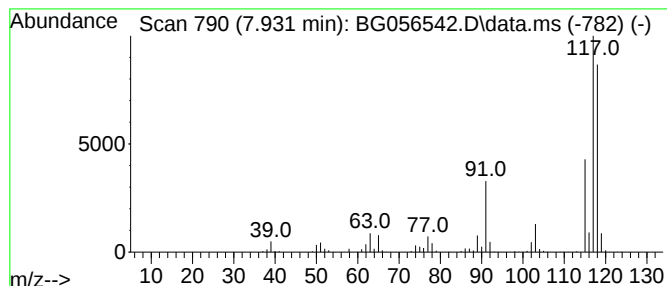
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzene, 1-ethenyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.931	299.86 ng	3509940	1,4-Dichlorobenzene-d4	8.272

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	96
2			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	95
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	93
5			Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	90



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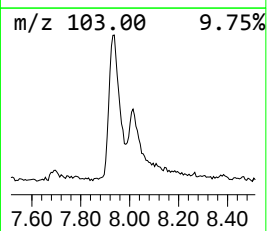
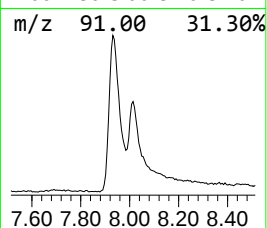
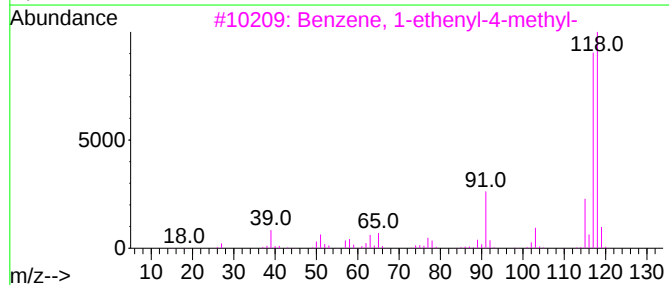
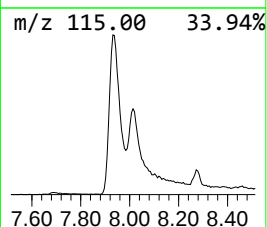
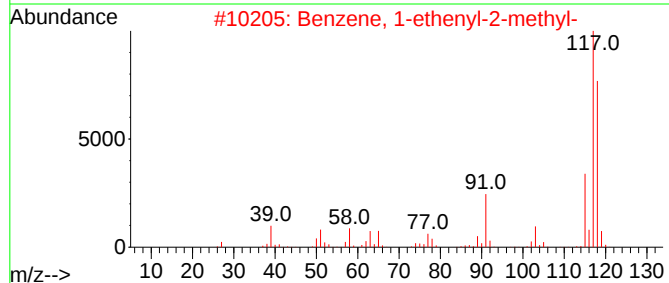
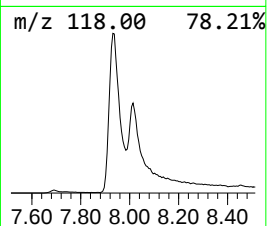
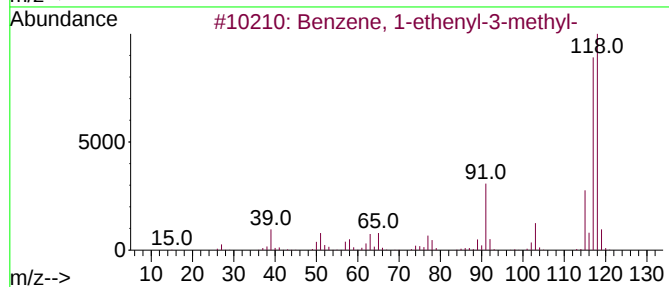
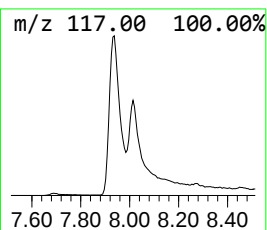
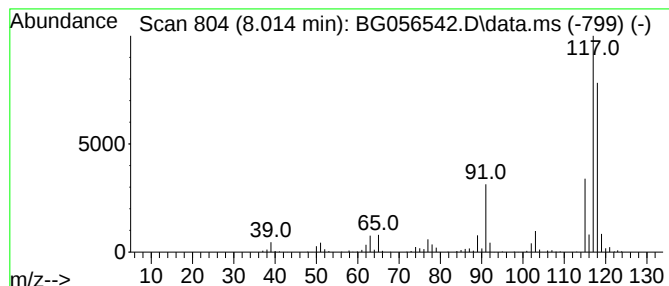
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, 1-ethenyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.014	186.19 ng	2179430	1,4-Dichlorobenzene-d4	8.272

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	95
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	95
3			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	93
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	90
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	90



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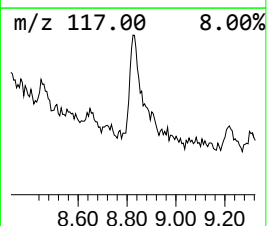
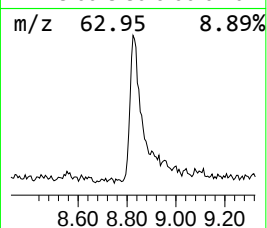
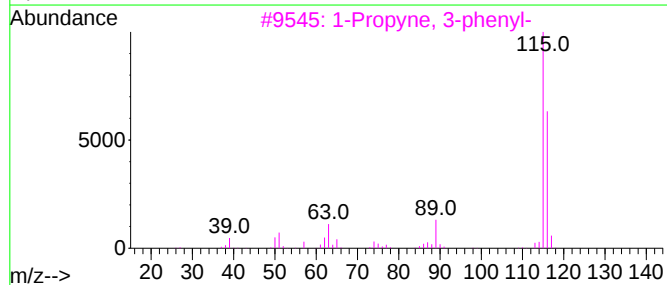
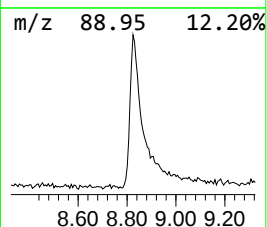
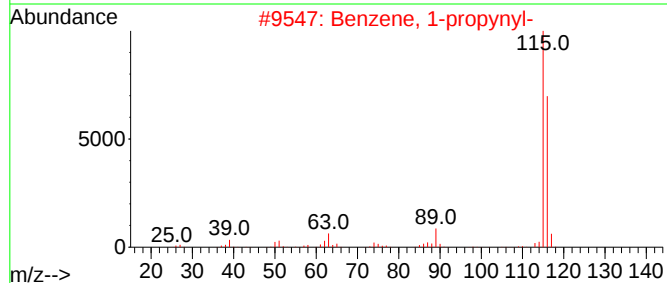
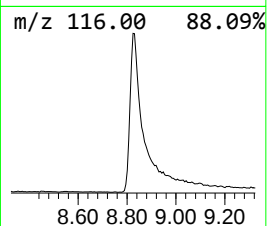
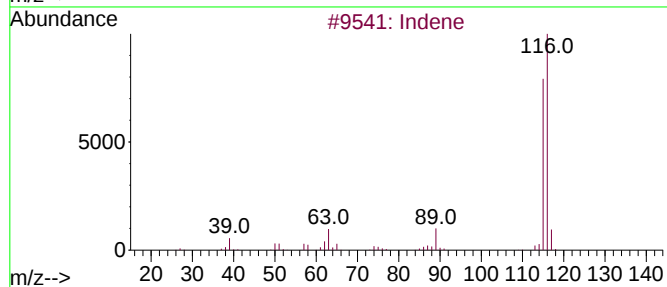
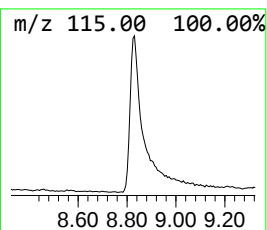
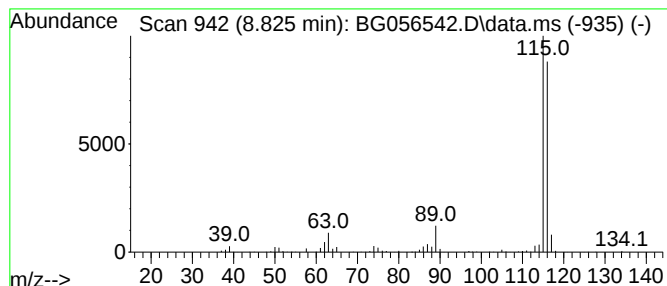
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Indene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.825	121.81 ng	1425800	1,4-Dichlorobenzene-d4	8.272

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	95
3			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	91
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

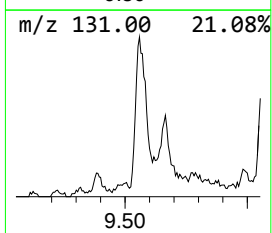
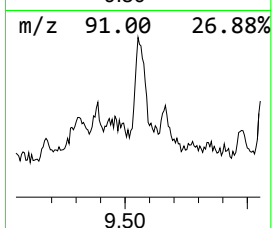
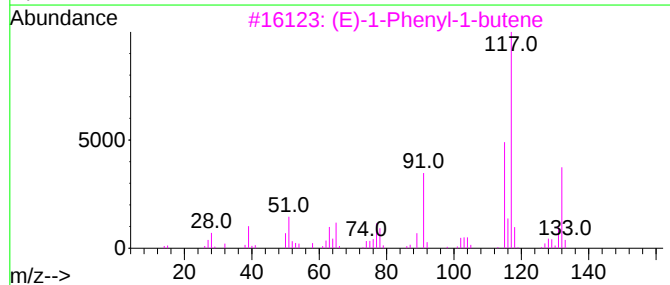
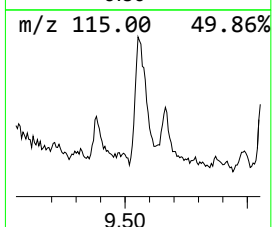
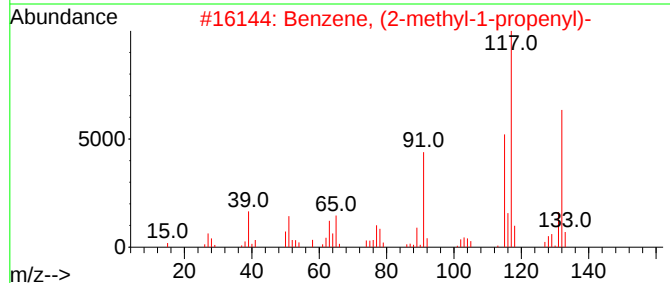
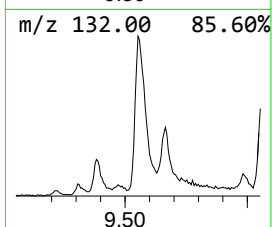
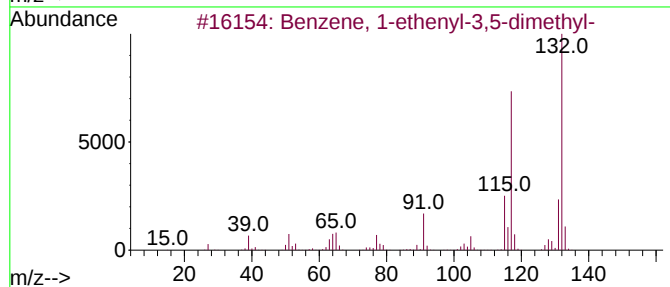
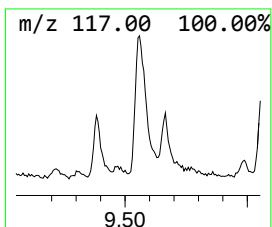
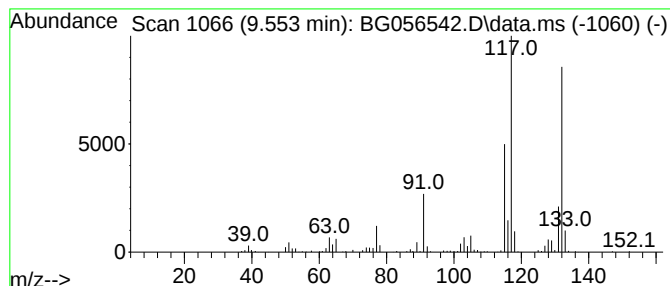
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, 1-ethenyl-3,5-dime... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.553	48.73 ng	570407	1,4-Dichlorobenzene-d4	8.272

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	95
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	94
3			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	94
4			o-Isopropenyltoluene	132	C10H12	007399-49-7	94
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
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Operator : CG/JU
Sample : 01348-03
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ALS Vial : 10 Sample Multiplier: 1

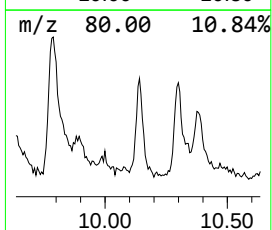
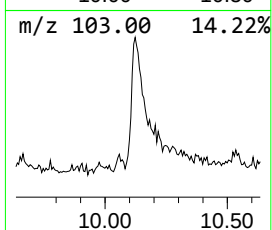
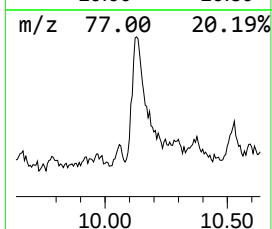
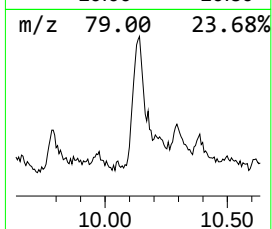
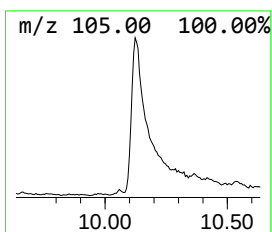
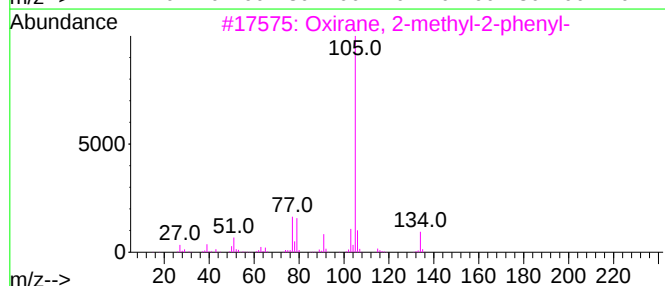
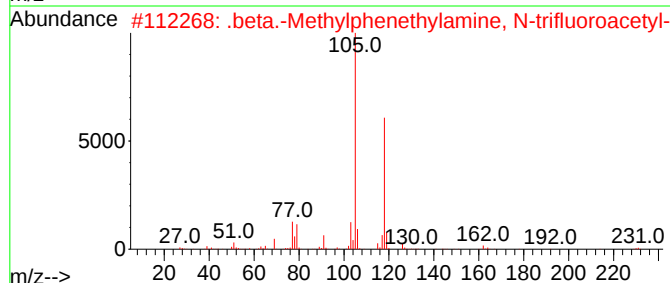
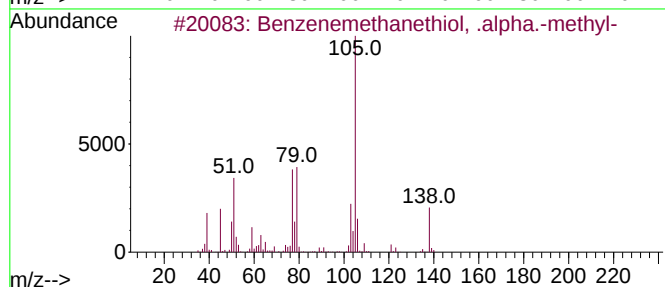
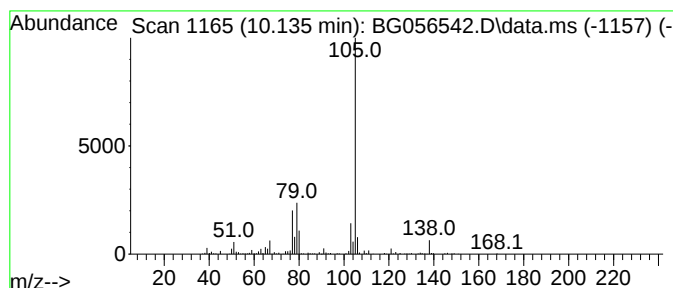
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzenemethanethiol, .alpha... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.135	50.25 ng	651379	Naphthalene-d8		11.110	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzenemethanethiol, .alpha.-met...		138	C8H10S	006263-65-6	68
2	.beta.-Methylphenethylamine, N-t...		231	C11H12F3NO	070414-02-7	64
3	Oxirane, 2-methyl-2-phenyl-		134	C9H10O	002085-88-3	64
4	Benzeneethanol, .beta.-methyl-		136	C9H12O	001123-85-9	59
5	Benzene, (1-methyl-3-butenyl)-		146	C11H14	010340-49-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
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Sample : 01348-03
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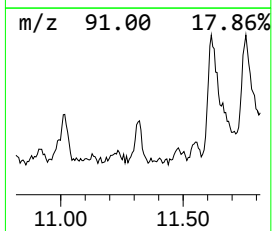
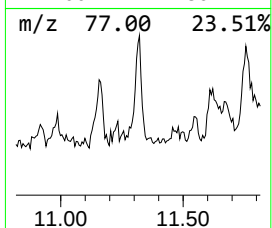
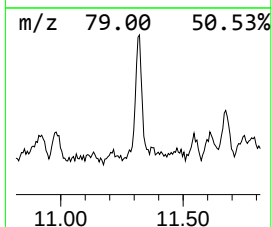
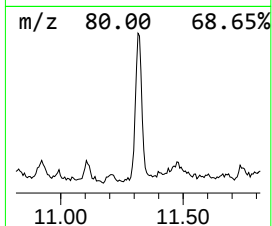
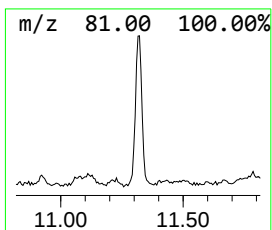
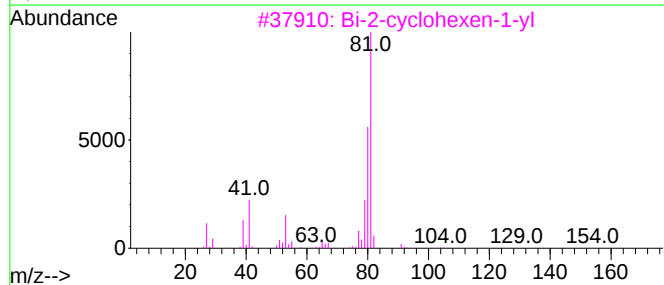
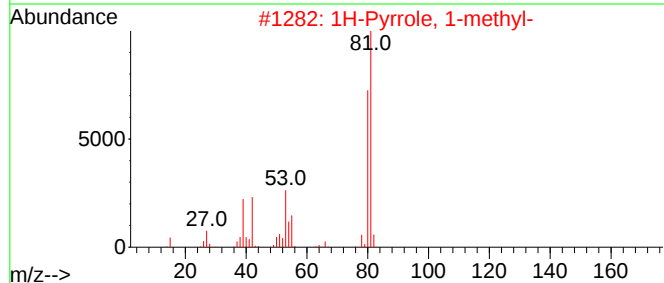
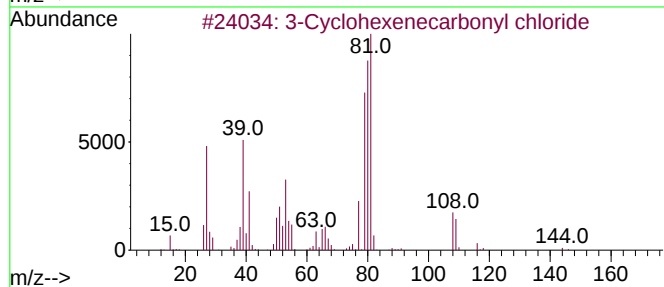
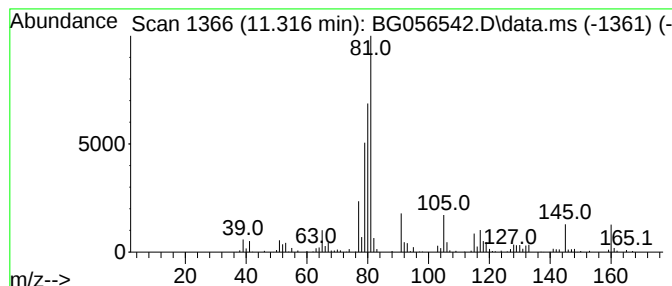
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Cyclohexenecarbonyl chloride Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.316	24.88 ng	322559	Naphthalene-d8	11.110	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclohexenecarbonyl chloride	144	C7H9ClO	000932-67-2	50
2	1H-Pyrrole, 1-methyl-	81	C5H7N	000096-54-8	43
3	Bi-2-cyclohexen-1-yl	162	C12H18	001541-20-4	40
4	Cyclobutane, 1,2-bis(1,3-butadie...	160	C12H16	080344-53-2	38
5	Cyclohexene, 1-bromo-	160	C6H9Br	002044-08-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
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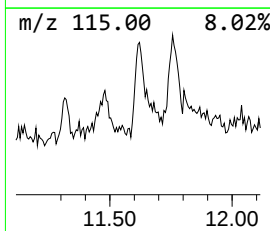
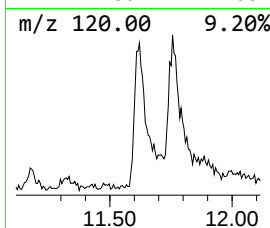
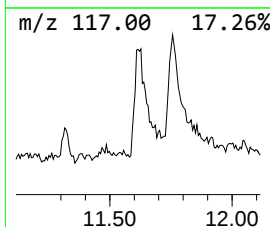
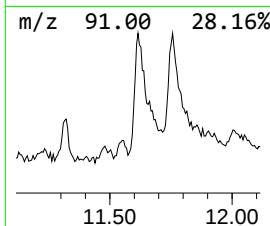
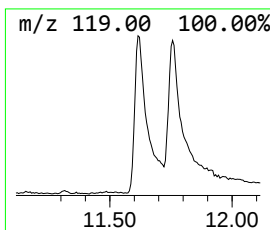
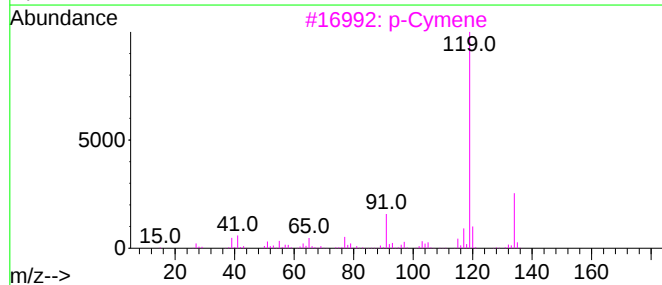
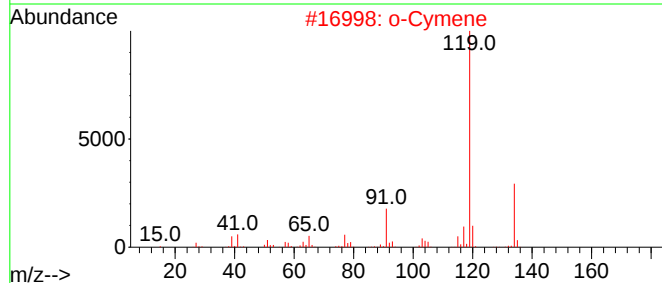
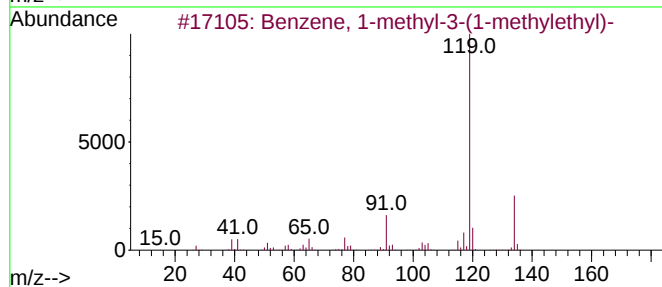
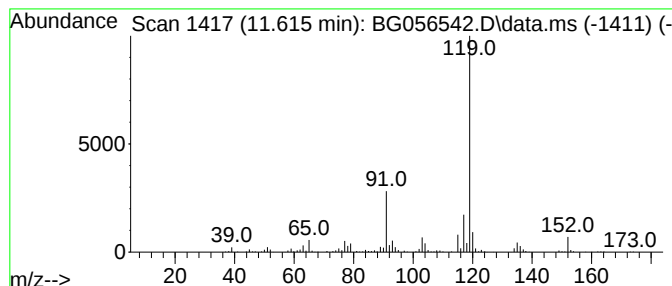
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ClientSampleId :
W-H5(31-32)

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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-methyl-3-(1-meth... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.615	42.68 ng	553199	Naphthalene-d8			11.110
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...		134	C10H14	000535-77-3	87
2	o-Cymene		134	C10H14	000527-84-4	81
3	p-Cymene		134	C10H14	000099-87-6	80
4	2,4-Dimethylbenzyl chloride		154	C9H11Cl	000824-55-5	72
5	Benzene, 1,2,3,5-tetramethyl-		134	C10H14	000527-53-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
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Sample : 01348-03
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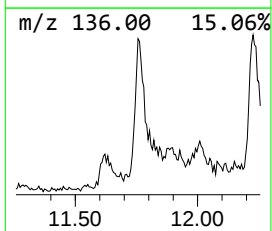
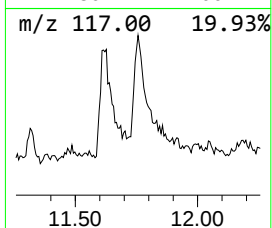
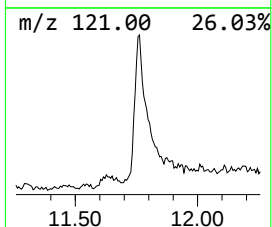
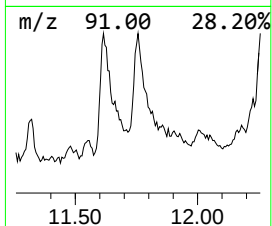
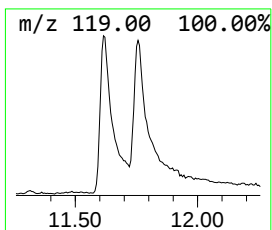
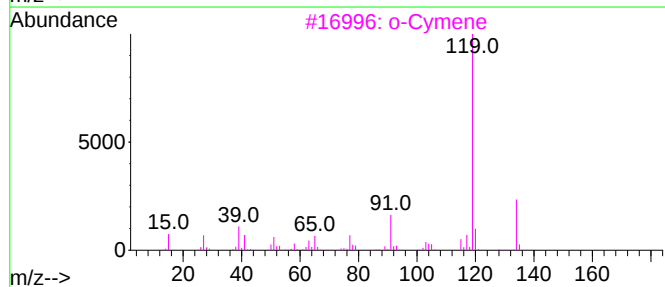
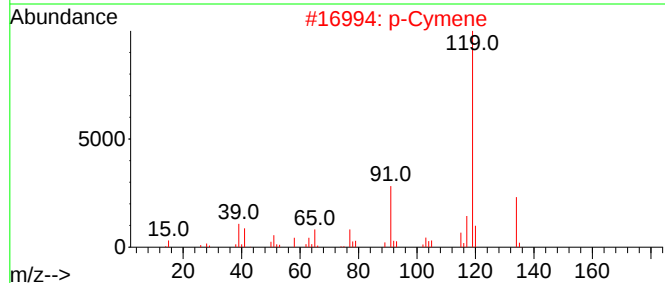
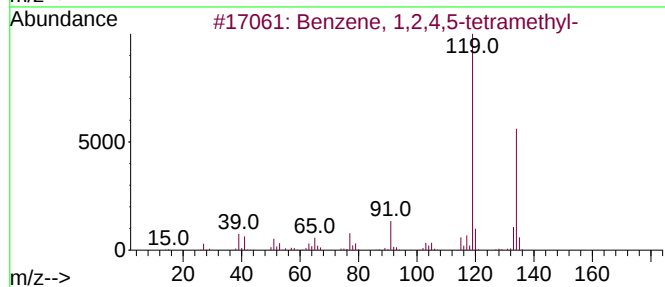
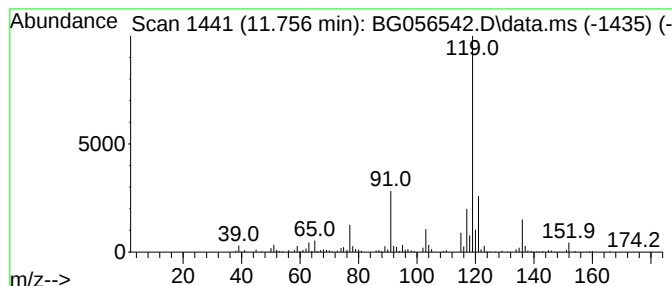
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W-H5(31-32)

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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 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.756	49.12 ng	636708	Naphthalene-d8	11.110	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
2	p-Cymene	134	C10H14	000099-87-6	64
3	o-Cymene	134	C10H14	000527-84-4	64
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	59
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
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Instrument :
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ClientSampleId :
W-H5(31-32)

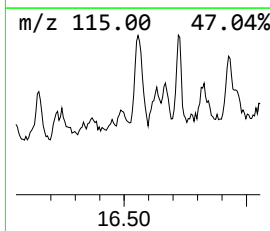
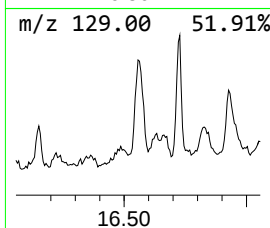
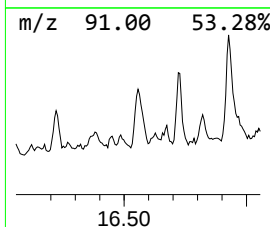
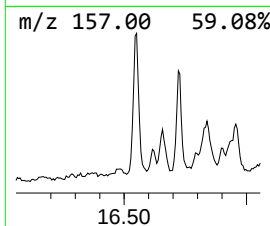
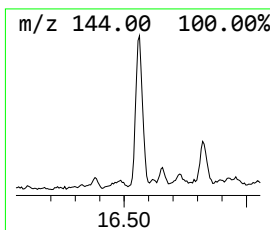
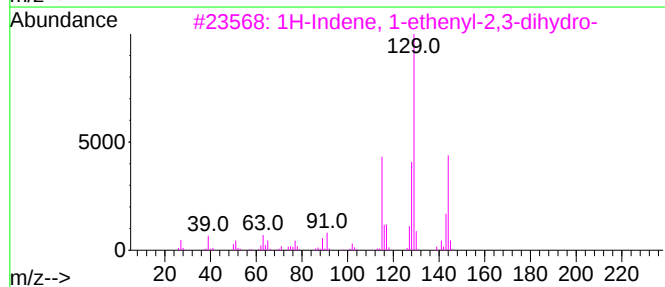
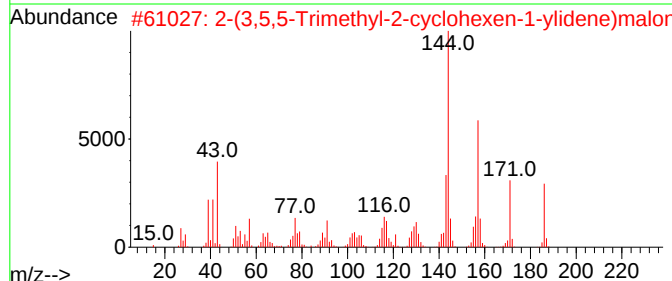
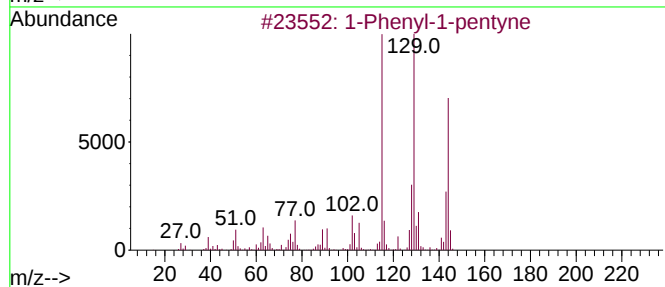
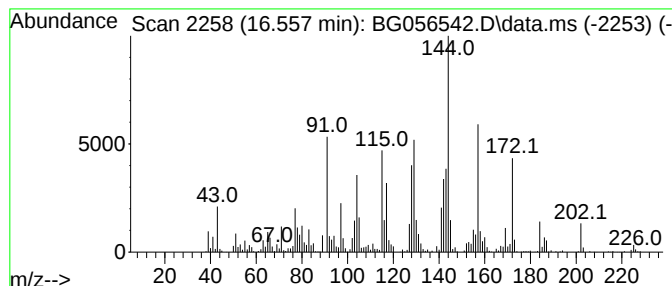
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.557 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.557	64.82 ng	1307290	Phenanthrene-d10	17.638

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-pentyne	144	C11H12	004250-81-1	46	
2	2-(3,5,5-Trimethyl-2-cyclohexen-...	186	C12H14N2	023051-44-7	45	
3	1H-Indene, 1-ethenyl-2,3-dihydro-	144	C11H12	051783-46-1	45	
4	Naphthalene, 1,2-dihydro-1,1,6-t...	172	C13H16	030364-38-6	42	
5	.alpha.-Methyl-2-naphthalenemeth...	172	C12H12O	007228-47-9	38	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :
W-H5(31-32)

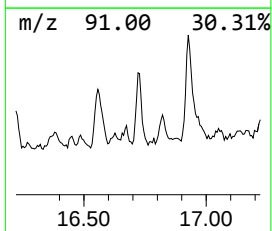
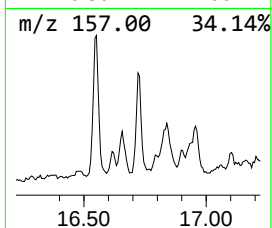
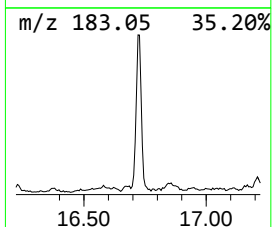
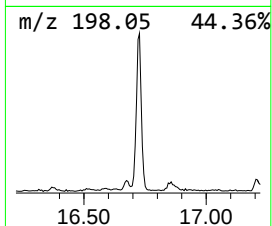
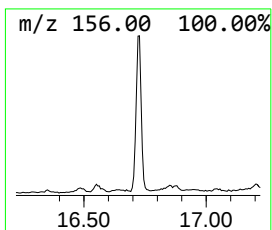
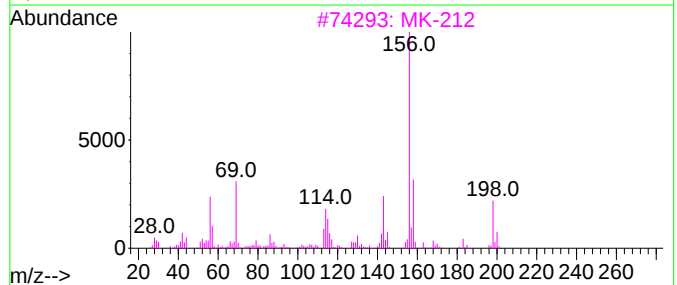
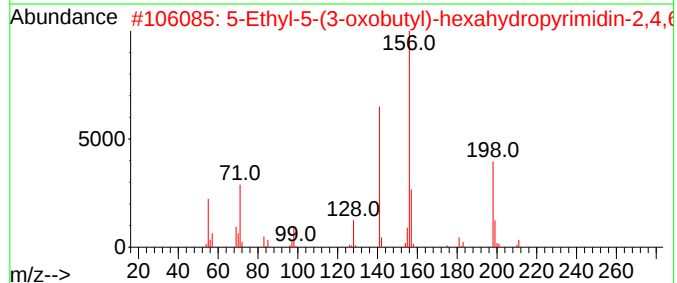
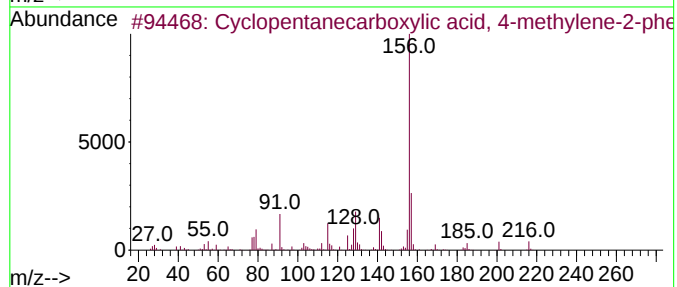
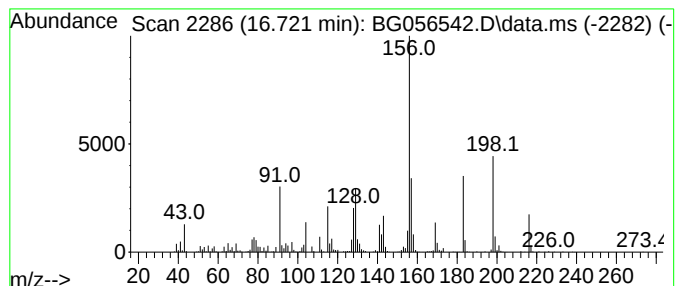
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.721 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.721	45.52 ng	917953	Phenanthrene-d10	17.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanecarboxylic acid, 4-m...	216	C14H16O2	074663-89-1	43
2			5-Ethyl-5-(3-oxobutyl)-hexahydro...	226	C10H14N2O4	1000281-56-8	40
3			MK-212	198	C8H11ClN4	064022-27-1	38
4			3H-1,2,4-Triazol-3-one, 2,4-diet...	171	C7H13N3O2	039636-06-1	35
5			Sulfone, phenyl 4-methylene-tran...	298	C18H18O2S	1000150-72-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

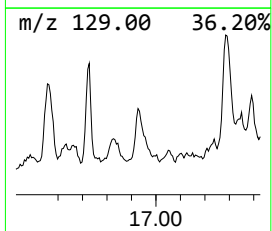
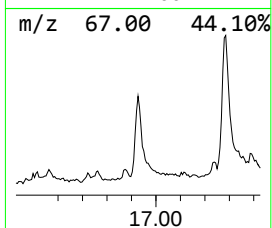
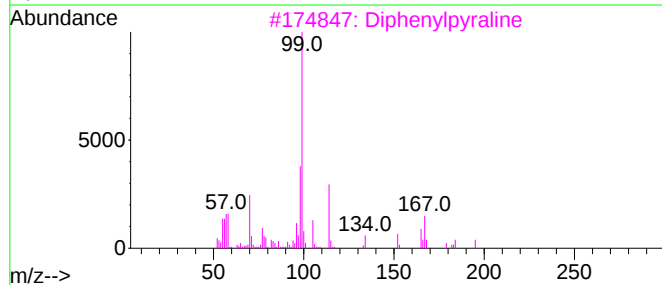
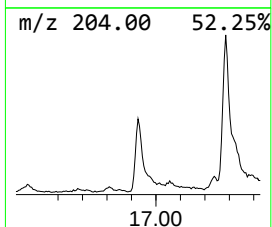
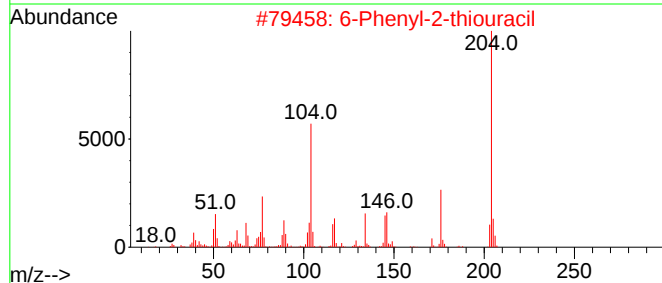
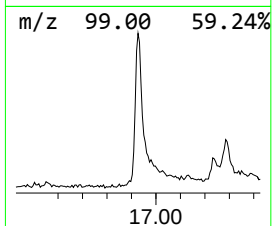
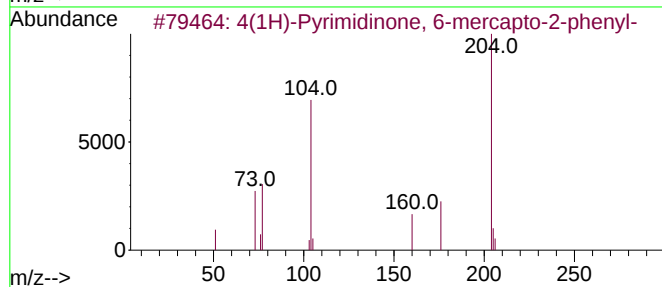
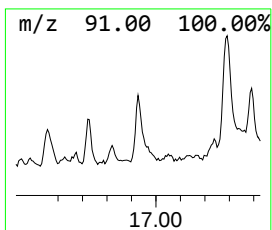
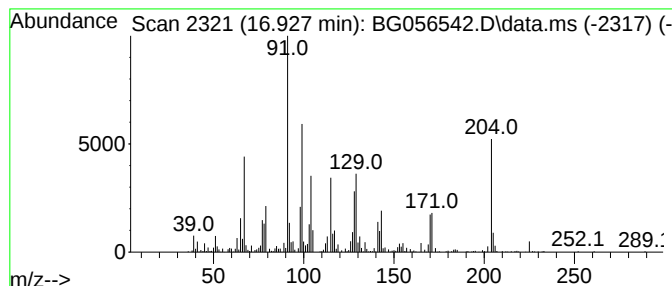
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.927 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.927	55.35 ng	1116310	Phenanthrene-d10	17.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4(1H)-Pyrimidinone, 6-mercapto-2...	204	C10H8N2OS	042956-81-0	11		
2	6-Phenyl-2-thiouracil	204	C10H8N2OS	005590-94-3	11		
3	Diphenylpyraline	281	C19H23NO	000147-20-6	10		
4	5-Nitro-3-p-tolyl-1H-[1,2,4]tria...	204	C9H8N4O2	1010296-48-9	10		
5	Histidine, N-trifluoacetyl-4-flu...	269	C8H7F4N3O3	1000116-45-1	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

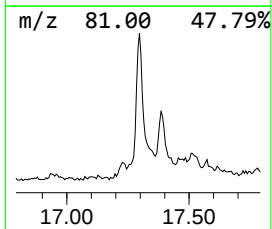
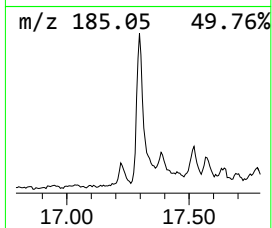
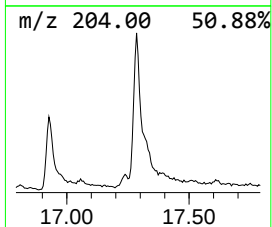
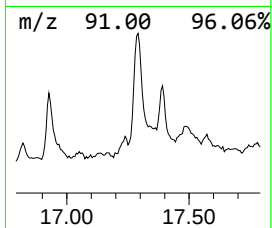
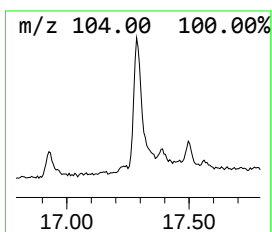
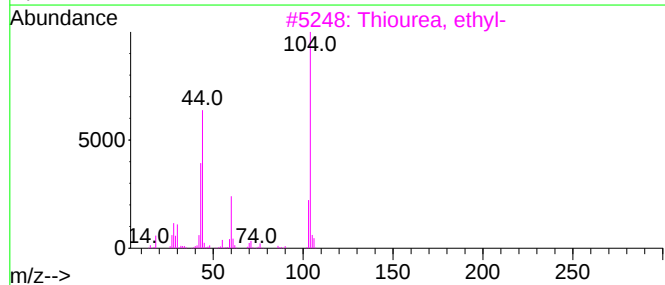
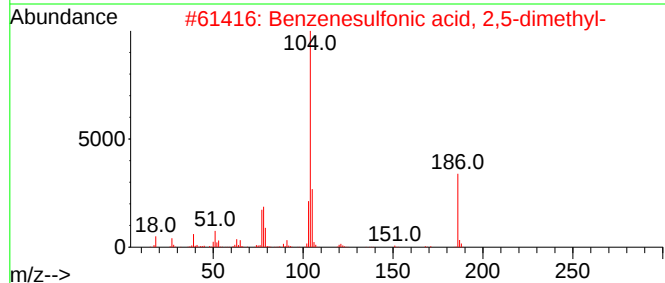
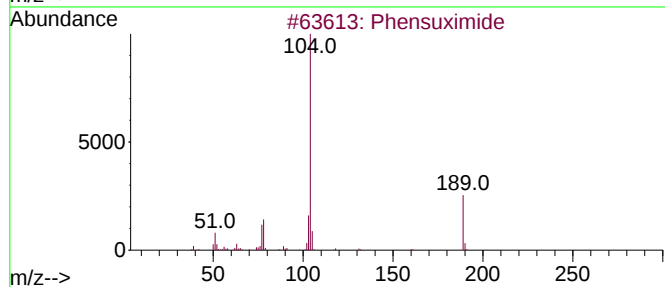
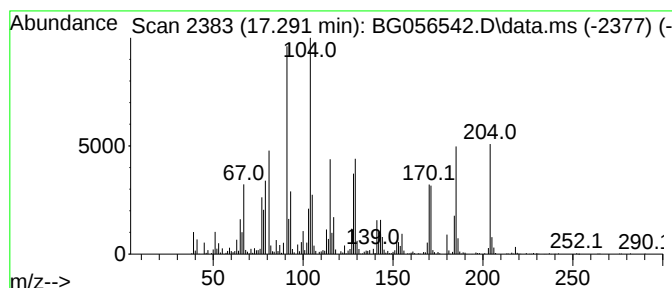
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.291 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.291	111.99 ng	2258470	Phenanthrene-d10	17.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phensuximide	189	C11H11NO2	000086-34-0	14
2			Benzenesulfonic acid, 2,5-dimethyl-	186	C8H10O3S	000609-54-1	14
3			Thiourea, ethyl-	104	C3H8N2S	000625-53-6	14
4			Benzene, 4-pentynyl-	144	C11H12	001823-14-9	14
5			Benzenemethanol, 2-methyl-, acetate	164	C10H12O2	017373-93-2	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

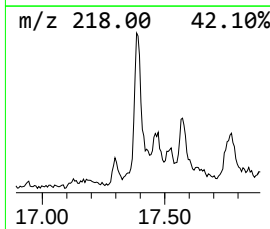
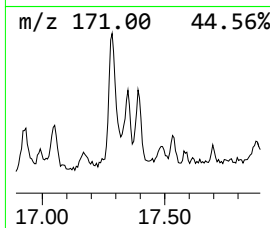
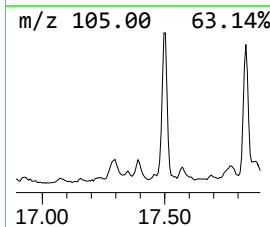
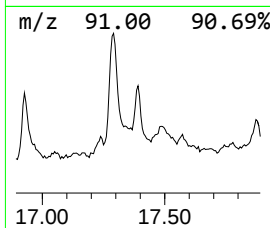
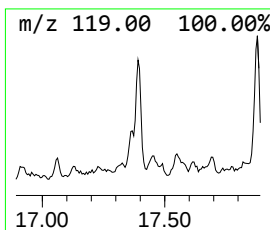
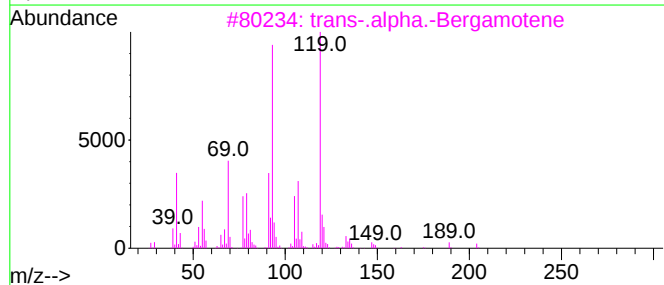
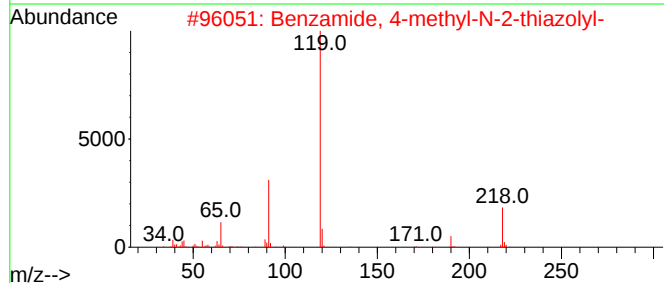
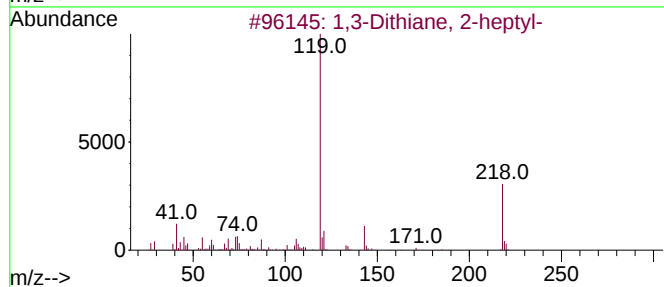
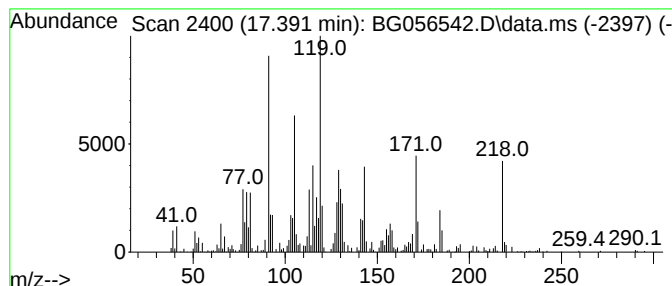
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown17.391 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.391	44.10 ng	889455	Phenanthrene-d10	17.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dithiane, 2-heptyl-	218	C11H22S2	059092-72-7	27
2			Benzamide, 4-methyl-N-2-thiazolyl-	218	C11H10N2OS	150175-93-2	22
3			trans-.alpha.-Bergamotene	204	C15H24	013474-59-4	11
4			benz[d]isoxazole, 3-ethyl-	147	C9H9NO	066033-77-0	11
5			Benzamide, 2-methyl-N-(2-ethoxyp...	255	C16H17NO2	055814-37-4	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

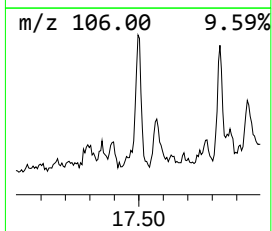
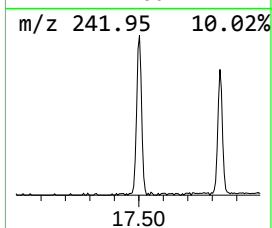
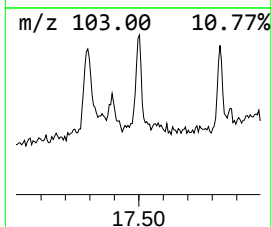
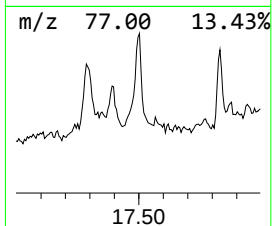
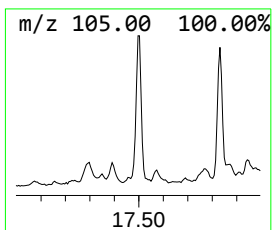
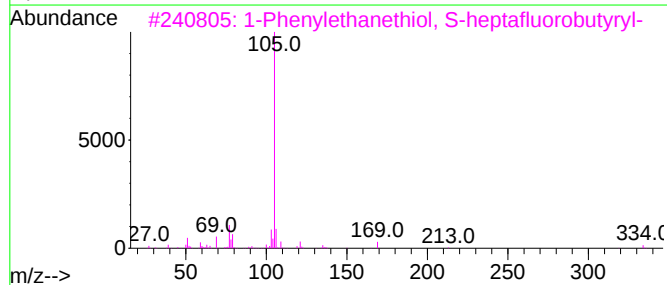
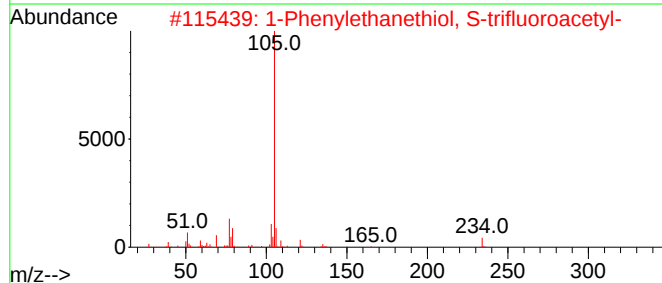
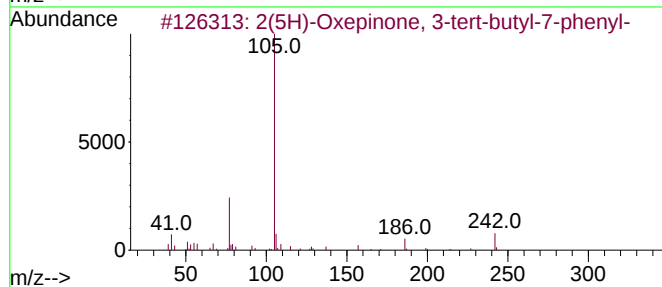
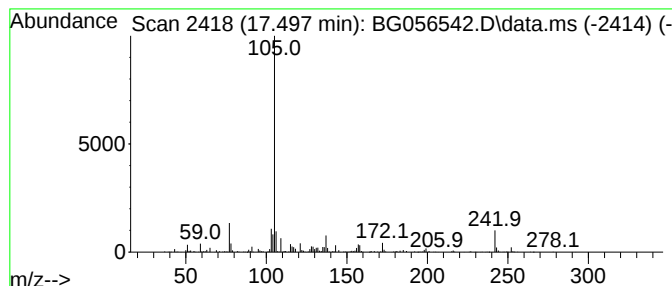
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown17.497 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.497	68.87 ng	1388810	Phenanthrene-d10	17.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(5H)-Oxepinone, 3-tert-butyl-7-...	242	C16H18O2	1000142-27-9	49		
2	1-Phenylethanethiol, S-trifluoro...	234	C10H9F3OS	1010469-38-4	47		
3	1-Phenylethanethiol, S-heptaflu...	334	C12H9F7OS	1000469-38-2	47		
4	1-Phenylethanethiol, S-pentaflu...	284	C11H9F5OS	1000469-38-3	47		
5	1-Phenylethanethiol, S-(2-methyl...	208	C12H16OS	1227931-65-8	47		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

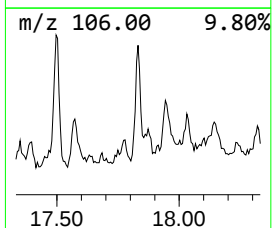
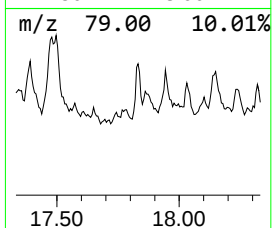
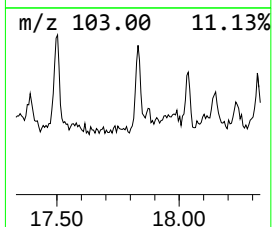
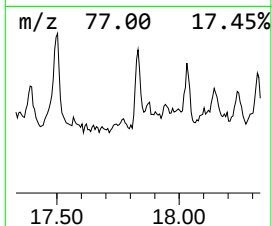
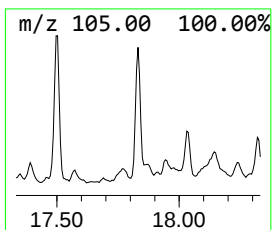
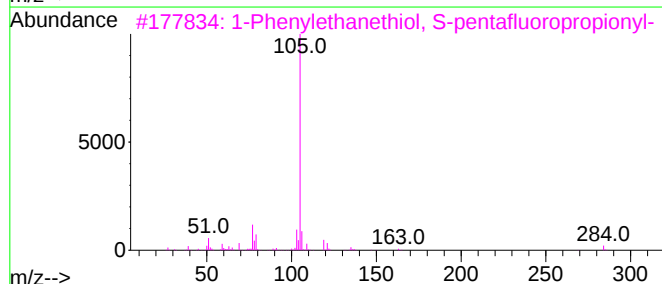
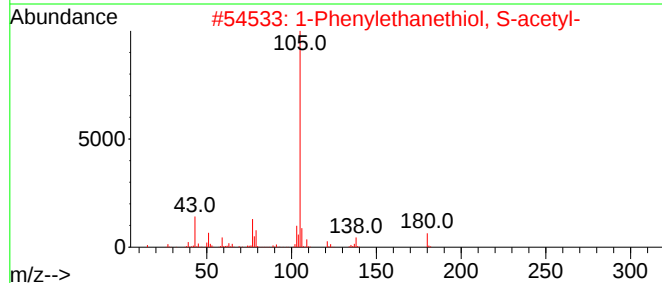
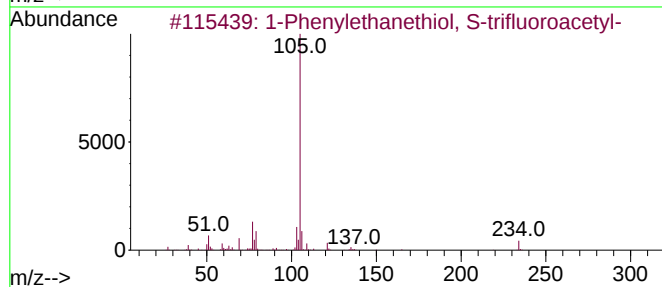
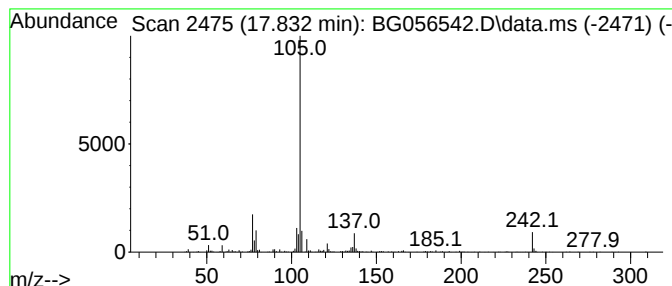
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 1-Phenylethanethiol, S-trif... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.832	28.02 ng	565117	Phenanthrene-d10	17.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenylethanethiol, S-trifluoro...	234	C10H9F3OS	1010469-38-4	74
2			1-Phenylethanethiol, S-acetyl-	180	C10H12OS	067385-07-3	72
3			1-Phenylethanethiol, S-pentafluo...	284	C11H9F5OS	1000469-38-3	64
4			2,4-Dimethylthiophenol	138	C8H10S	013616-82-5	64
5			Benzenemethanethiol, .alpha.-met...	138	C8H10S	006263-65-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

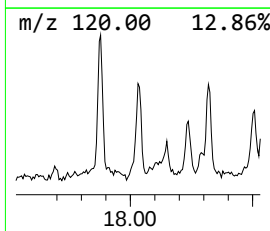
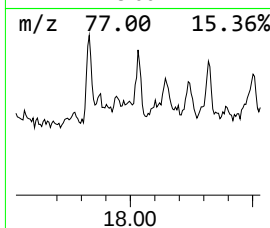
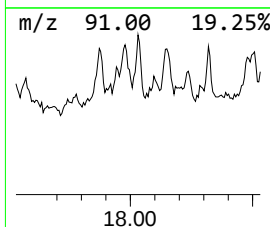
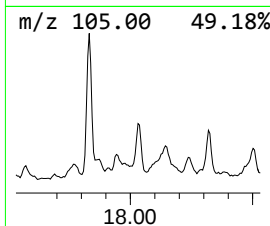
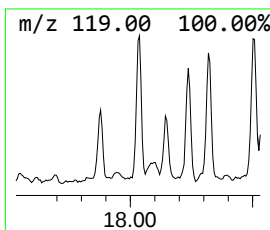
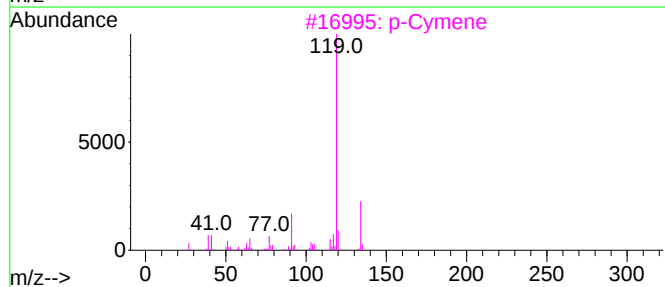
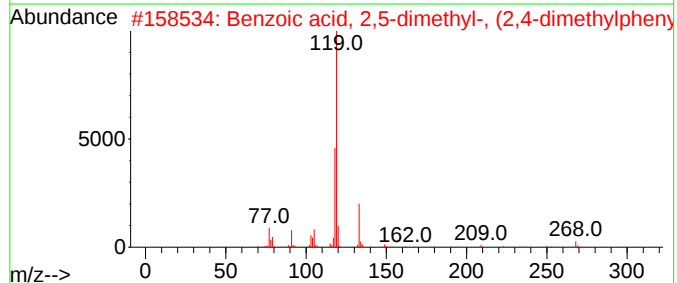
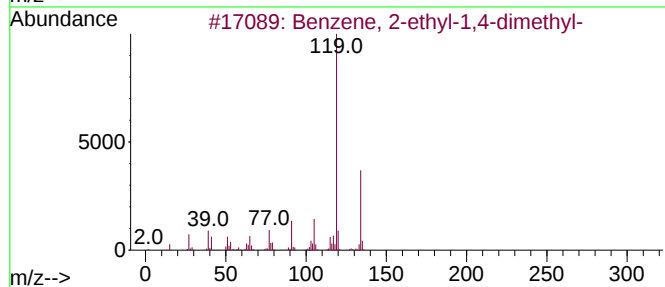
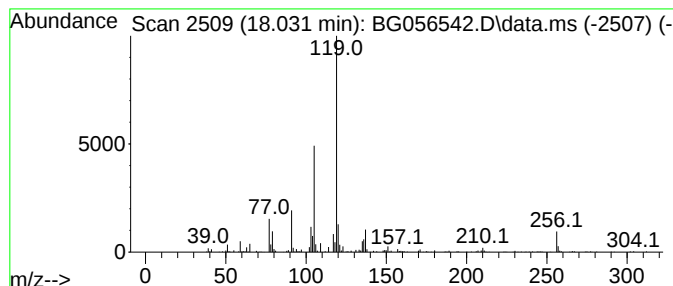
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W-H5(31-32)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.031	27.56 ng	555738	Phenanthrene-d10	17.638	
Hit#	of 5	Tentative ID	MW MolForm	CAS#	Qual
1		Benzene, 2-ethyl-1,4-dimethyl-	134 C10H14	001758-88-9	59
2		Benzoic acid, 2,5-dimethyl-, (2,...	268 C18H20O2	055000-48-1	59
3		p-Cymene	134 C10H14	000099-87-6	59
4		o-Cymene	134 C10H14	000527-84-4	59
5		Benzene, 4-ethyl-1,2-dimethyl-	134 C10H14	000934-80-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

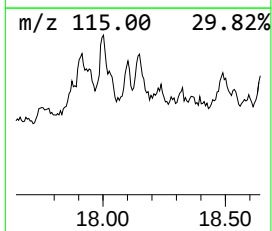
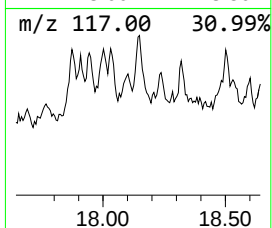
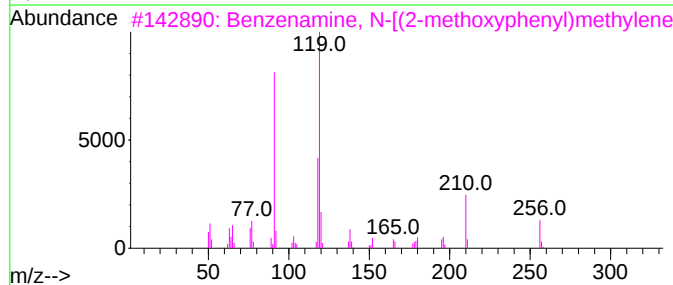
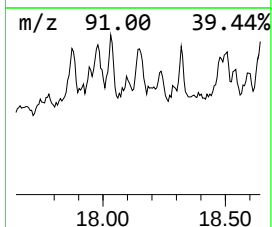
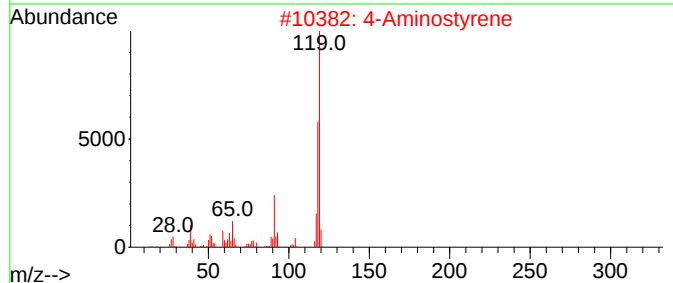
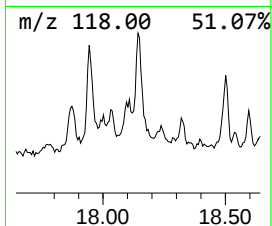
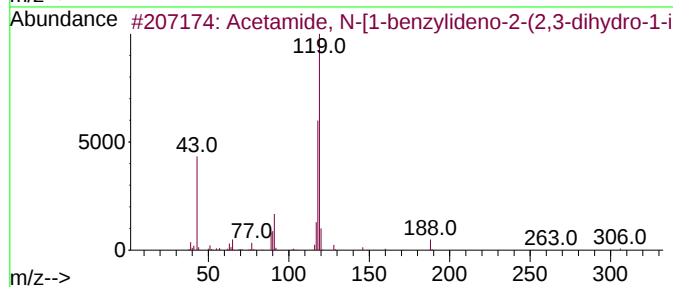
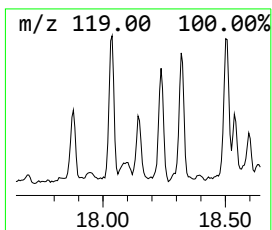
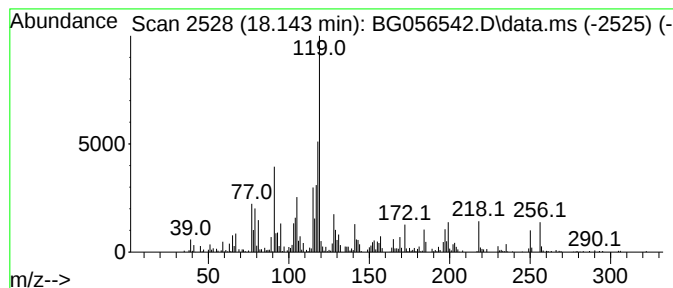
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown18.143 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.143	36.98 ng	745719	Phenanthrene-d10	17.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetamide, N-[1-benzylideno-2-(2...	306	C19H18N2O2	314281-76-0	47
2			4-Aminostyrene	119	C8H9N	001520-21-4	47
3			Benzenamine, N-[(2-methoxyphenyl)...]	256	C14H12N2O3	024588-82-7	43
4			9-Borabicyclo[3.3.1]nonane, 9-(2...	256	C17H25BO	1010161-02-3	43
5			3-Methylbenzoic acid, 3-fluoroph...	230	C14H11FO2	1000331-26-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

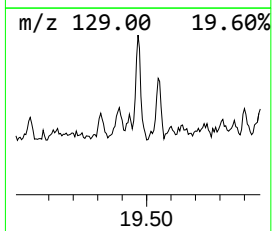
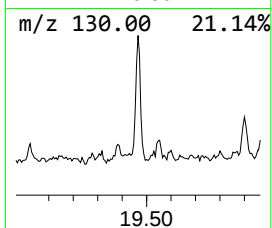
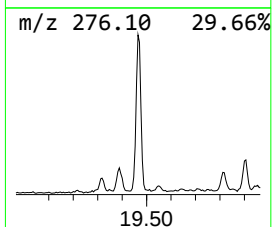
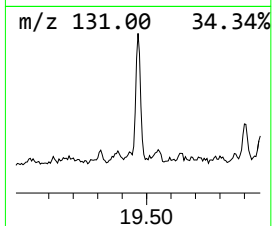
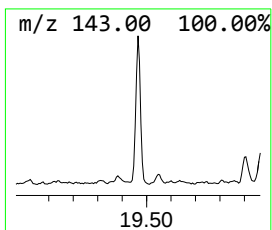
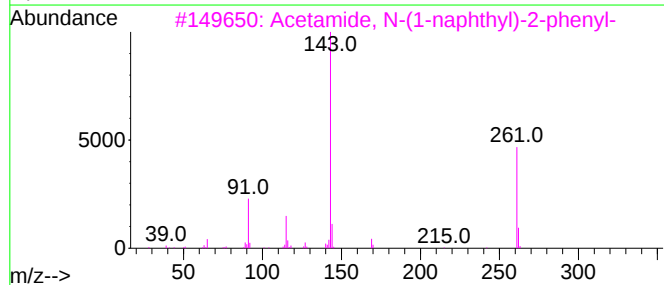
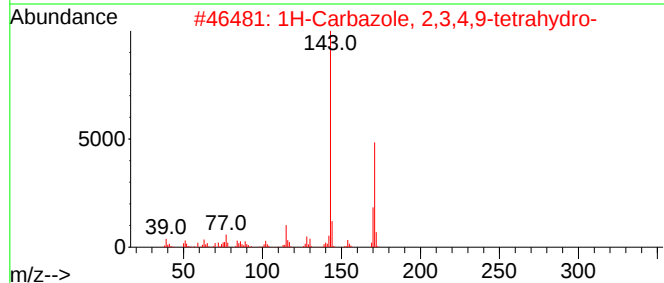
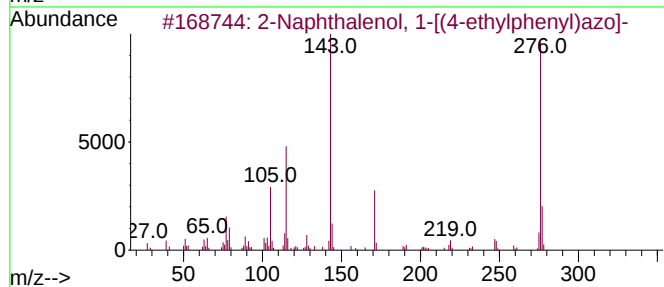
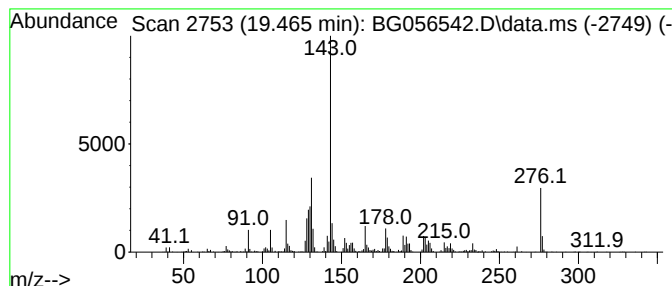
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown19.465 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.465	64.38 ng	1298320	Phenanthrene-d10	17.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Naphthalenol, 1-[(4-ethylpheny...	276	C18H16N2O	050607-58-4	43		
2	1H-Carbazole, 2,3,4,9-tetrahydro-	171	C12H13N	000942-01-8	38		
3	Acetamide, N-(1-naphthyl)-2-phenyl-	261	C18H15NO	1000307-14-9	38		
4	Quinoline, 6-methyl-	143	C10H9N	000091-62-3	30		
5	1-Methyl-1-(2-pentyloxy)-1-silac...	186	C10H22OSi	1000216-95-9	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

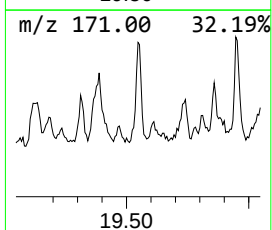
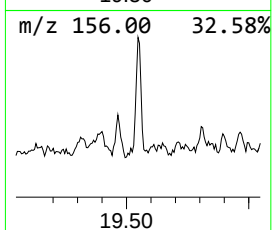
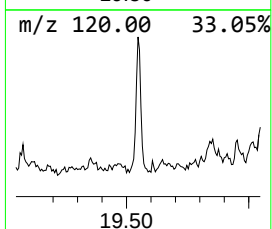
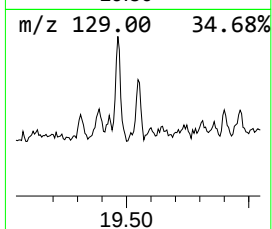
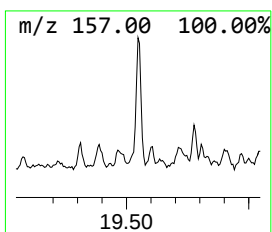
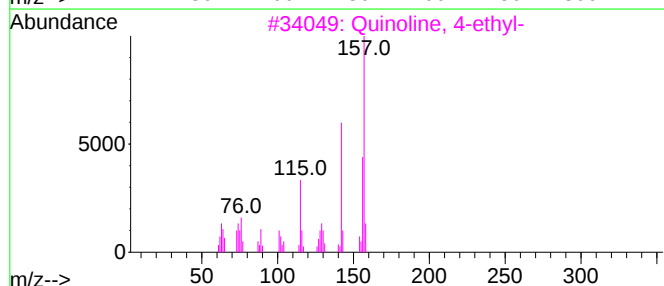
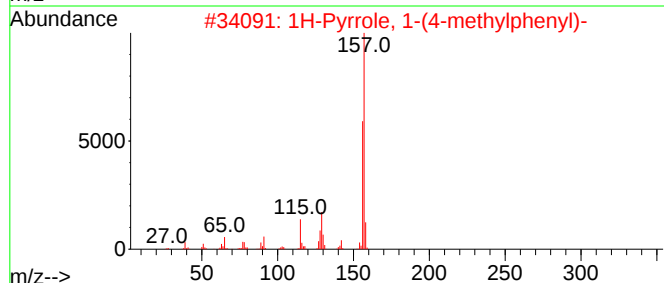
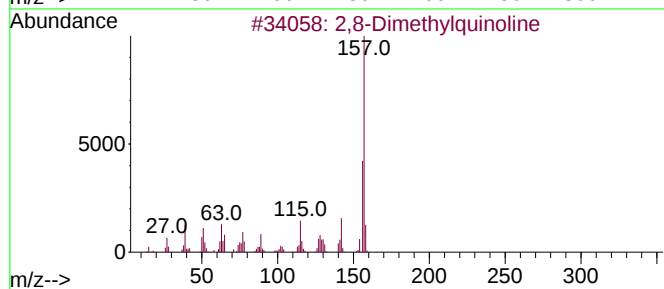
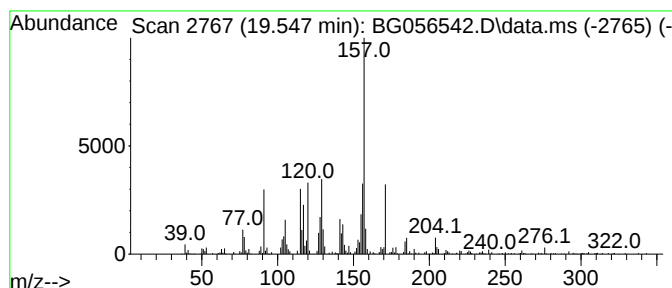
Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 2,8-Dimethylquinoline Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.547	27.29 ng	550329	Phenanthrene-d10		17.638	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,8-Dimethylquinoline		157	C11H11N	001463-17-8	50
2	1H-Pyrrole, 1-(4-methylphenyl)-		157	C11H11N	000827-60-1	50
3	Quinoline, 4-ethyl-		157	C11H11N	019020-26-9	49
4	Quinoline, 4,8-dimethyl-		157	C11H11N	013362-80-6	49
5	Quinoline, 2,6-dimethyl-		157	C11H11N	000877-43-0	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020323\
Data File : BG056542.D
Acq On : 3 Feb 2023 17:11
Operator : CG/JU
Sample : 01348-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
W-H5(31-32)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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
Bicyclo[4.2.0]o...	6.233	369.5	ng	4325230	1	8.272	234107	20.0
Benzene, 1-ethe...	7.931	299.9	ng	3509940	1	8.272	234107	20.0
Benzene, 1-ethe...	8.014	186.2	ng	2179430	1	8.272	234107	20.0
Indene	8.825	121.8	ng	1425800	1	8.272	234107	20.0
Benzene, 1-ethe...	9.553	48.7	ng	570407	1	8.272	234107	20.0
Benzenemethanet...	10.135	50.3	ng	651379	2	11.110	259260	20.0
3-Cyclohexeneca...	11.316	24.9	ng	322559	2	11.110	259260	20.0
Benzene, 1-meth...	11.615	42.7	ng	553199	2	11.110	259260	20.0
Benzene, 1,2,4,...	11.756	49.1	ng	636708	2	11.110	259260	20.0
unknown16.557	16.557	64.8	ng	1307290	4	17.638	403337	20.0
unknown16.721	16.721	45.5	ng	917953	4	17.638	403337	20.0
unknown16.927	16.927	55.4	ng	1116310	4	17.638	403337	20.0
unknown17.291	17.291	112.0	ng	2258470	4	17.638	403337	20.0
unknown17.391	17.391	44.1	ng	889455	4	17.638	403337	20.0
unknown17.497	17.497	68.9	ng	1388810	4	17.638	403337	20.0
1-Phenylethanet...	17.832	28.0	ng	565117	4	17.638	403337	20.0
Benzene, 2-ethy...	18.031	27.6	ng	555738	4	17.638	403337	20.0
unknown18.143	18.143	37.0	ng	745719	4	17.638	403337	20.0
unknown19.465	19.465	64.4	ng	1298320	4	17.638	403337	20.0
2,8-Dimethylqui...	19.547	27.3	ng	550329	4	17.638	403337	20.0