

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
 Data File : BG060044.D
 Acq On : 15 Dec 2023 20:34
 Operator : MA/JU
 Sample : 05688-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-3

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-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060044.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.142	4	9	25	rVB	598849	1095645	15.26%	2.849%
2	4.152	176	181	185	rBV2	48336	75602	1.05%	0.197%
3	4.464	231	234	243	rBV3	61242	95835	1.33%	0.249%
4	5.022	325	329	334	rBV2	44352	78706	1.10%	0.205%
5	5.145	346	350	358	rVB8	36931	76072	1.06%	0.198%
6	5.527	409	415	422	rBV	469677	761590	10.60%	1.980%
7	5.598	422	427	430	rBV2	394251	726935	10.12%	1.890%
8	5.968	484	490	500	rBV	400399	684760	9.53%	1.781%
9	7.043	666	673	678	rBV	210564	350335	4.88%	0.911%
10	7.108	678	684	692	rVV2	400177	713553	9.94%	1.855%
11	7.178	692	696	704	rVB	111293	185508	2.58%	0.482%
12	7.349	718	725	737	rVB	307759	514139	7.16%	1.337%
13	7.601	762	768	777	rVB	390201	669862	9.33%	1.742%
14	7.960	822	829	834	rBV	233074	415085	5.78%	1.079%
15	8.071	842	848	858	rVB	171394	319186	4.44%	0.830%
16	8.224	868	874	881	rBV	233819	399185	5.56%	1.038%
17	8.330	885	892	898	rBV	67852	112492	1.57%	0.293%
18	8.447	907	912	917	rBV3	58127	94582	1.32%	0.246%
19	8.500	917	921	927	rVB3	49277	84729	1.18%	0.220%
20	8.594	932	937	941	rVV3	113913	195469	2.72%	0.508%
21	8.635	941	944	951	rVB3	98795	165983	2.31%	0.432%
22	8.770	959	967	974	rBV	249932	493889	6.88%	1.284%
23	8.911	986	991	995	rBV	79138	114790	1.60%	0.298%
24	8.964	995	1000	1005	rVB	61994	94442	1.31%	0.246%
25	9.064	1011	1017	1021	rBV	227763	378816	5.27%	0.985%
26	9.117	1021	1026	1039	rVB2	635456	1344257	18.72%	3.495%
27	9.399	1068	1074	1080	rBV4	42615	78375	1.09%	0.204%
28	9.587	1100	1106	1111	rBV2	103029	163927	2.28%	0.426%
29	9.646	1111	1116	1123	rVV	84708	130867	1.82%	0.340%
30	10.010	1172	1178	1183	rVV	52816	89394	1.24%	0.232%
31	10.163	1196	1204	1211	rBV3	186596	388233	5.41%	1.010%
32	10.339	1225	1234	1240	rBV2	51598	103724	1.44%	0.270%
33	10.451	1248	1253	1261	rVB3	126445	225824	3.14%	0.587%
34	10.674	1285	1291	1296	rBV	164541	281845	3.92%	0.733%
35	10.762	1296	1306	1311	rVV	339155	708830	9.87%	1.843%
36	10.809	1311	1314	1320	rVV6	54459	111473	1.55%	0.290%

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Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.874	1320	1325	1330	rVB2	51916	79492	1.11%	0.207%
38	12.137	1530	1540	1554	rVB3	401449	752745	10.48%	1.957%
39	12.478	1591	1598	1603	rBV2	74048	117951	1.64%	0.307%
40	12.572	1608	1614	1618	rBV2	44858	75107	1.05%	0.195%
41	13.218	1716	1724	1735	rBV	1981749	3059182	42.60%	7.955%
42	13.718	1802	1809	1812	rBV4	45524	83751	1.17%	0.218%
43	13.759	1812	1816	1822	rVB2	121477	194375	2.71%	0.505%
44	14.593	1951	1958	1966	rBV	611600	928423	12.93%	2.414%
45	16.079	2204	2211	2221	rBV	2035103	3031403	42.21%	7.883%
46	17.343	2419	2426	2431	rBV	963471	1423855	19.83%	3.702%
47	18.230	2572	2577	2588	rBV3	239593	343519	4.78%	0.893%
48	19.505	2788	2794	2801	rBV4	75852	117815	1.64%	0.306%
49	19.963	2865	2872	2881	rBV	5579504	7181966	100.00%	18.675%
50	21.262	3089	3093	3100	rBV2	157445	235180	3.27%	0.612%
51	21.608	3145	3152	3165	rBV2	1237858	2142824	29.84%	5.572%
52	22.396	3281	3286	3293	rBV2	149128	273089	3.80%	0.710%
53	23.271	3428	3435	3446	rVB3	221287	551716	7.68%	1.435%
54	24.317	3604	3613	3624	rBV2	240451	653737	9.10%	1.700%
55	24.805	3684	3696	3708	rBV2	748576	2163966	30.13%	5.627%
56	25.609	3822	3833	3845	rBV5	217874	777578	10.83%	2.022%
57	27.219	4097	4107	4123	rVB5	198868	764916	10.65%	1.989%
58	29.258	4439	4454	4469	rBV7	149456	771015	10.74%	2.005%
59	31.814	4878	4889	4890	rBV6	84783	209372	2.92%	0.544%

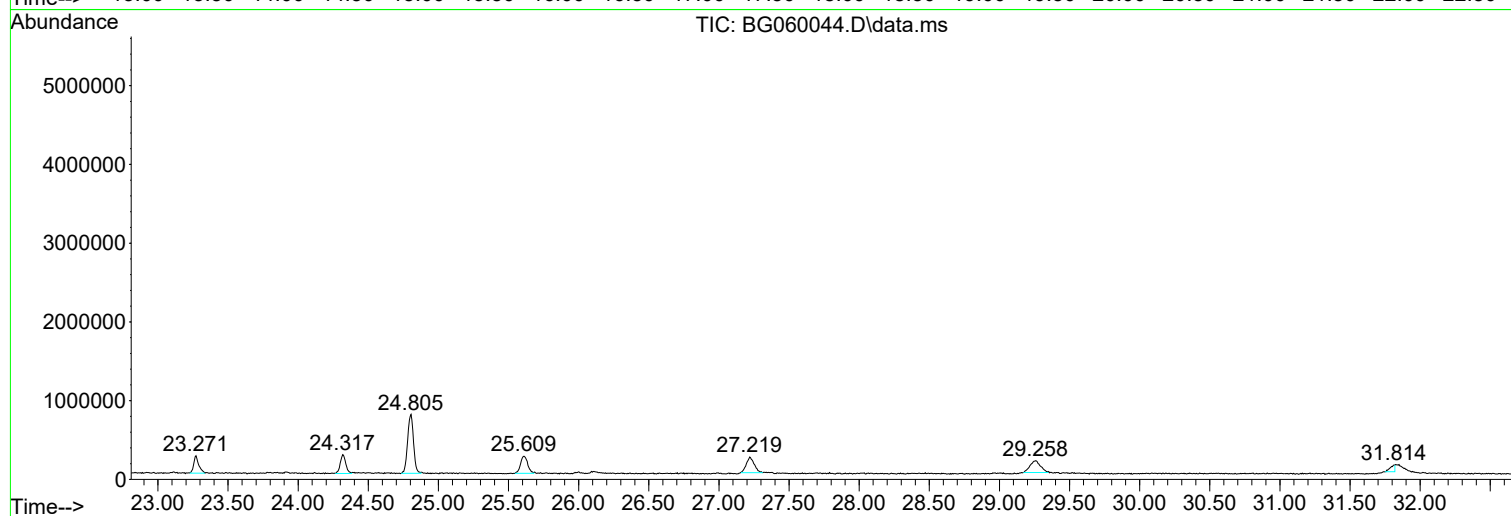
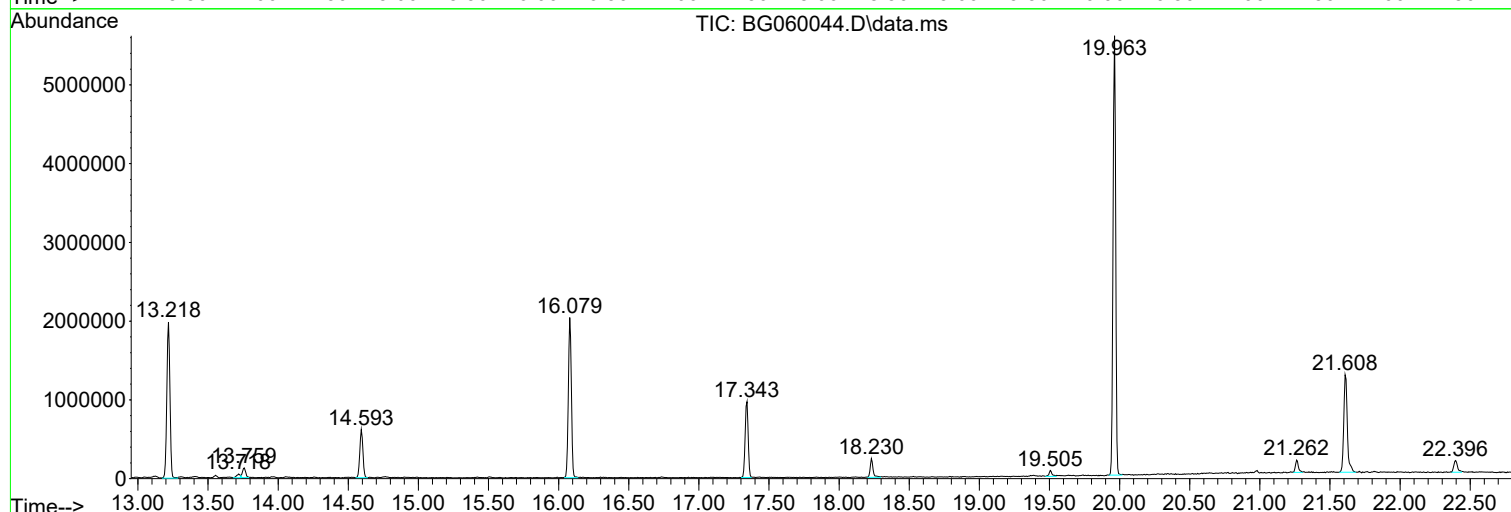
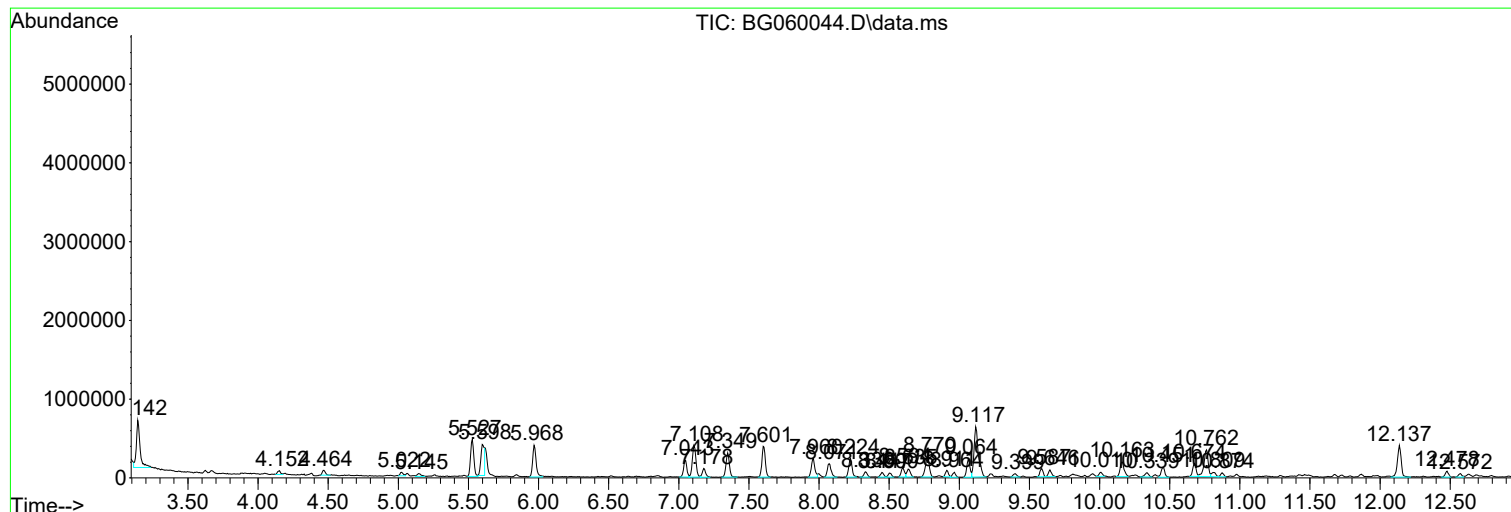
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : 05688-04
Misc :
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Instrument :
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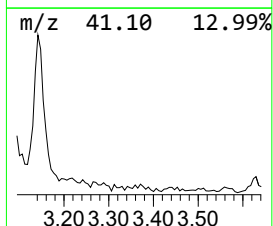
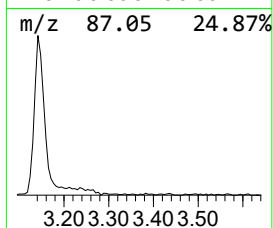
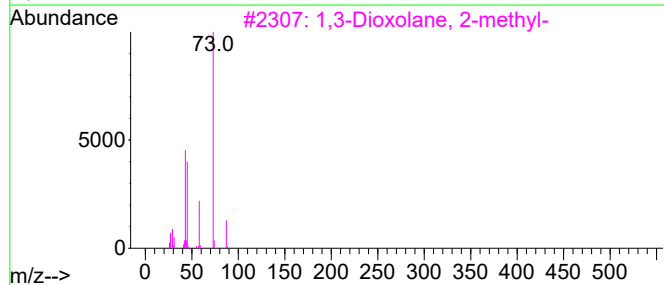
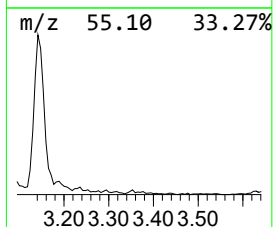
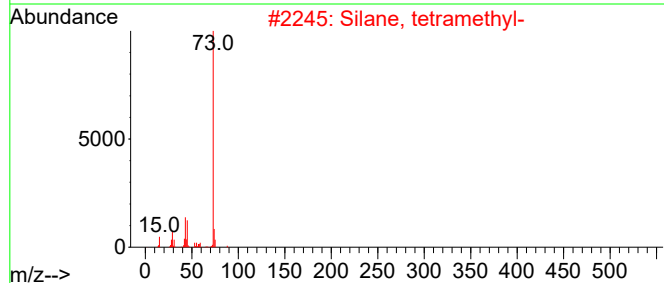
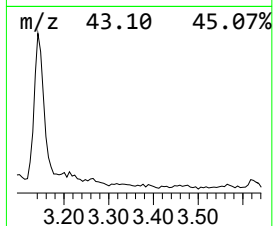
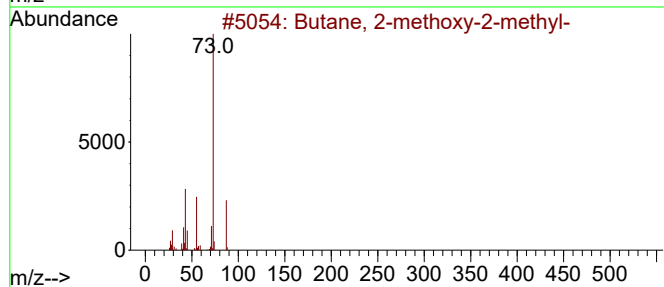
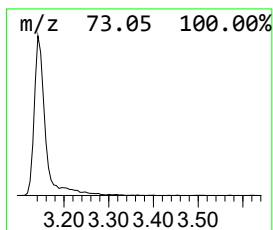
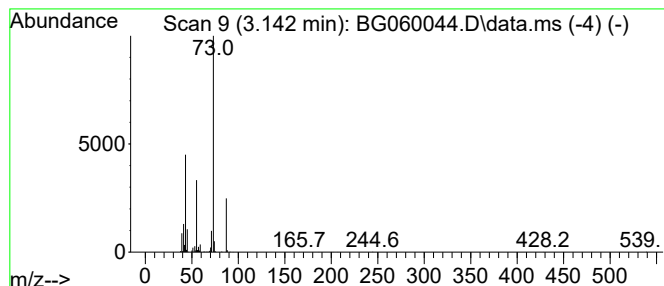
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.142	52.79 ng	1095650	1,4-Dichlorobenzene-d4	7.954

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9



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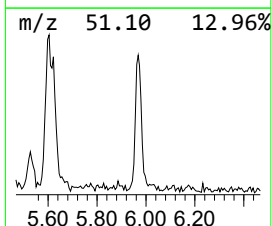
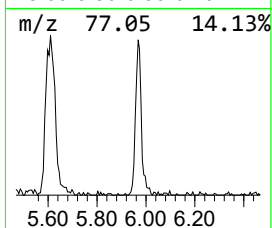
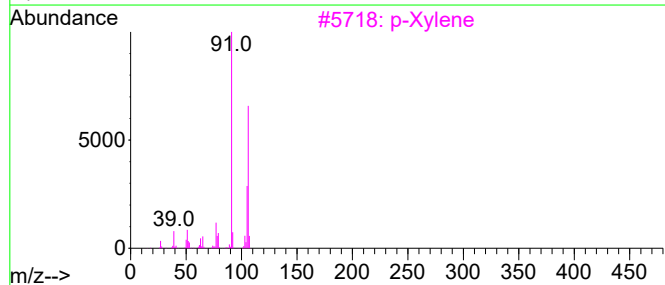
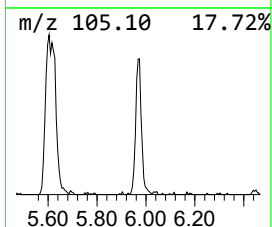
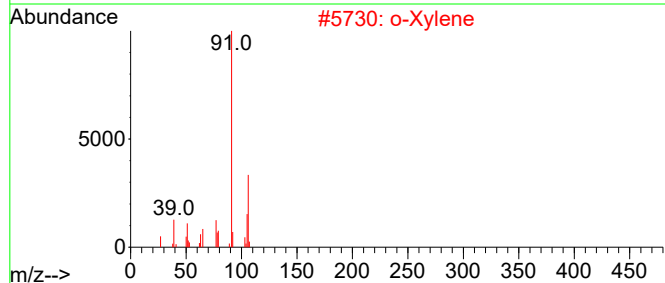
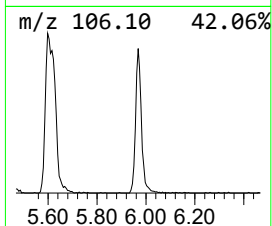
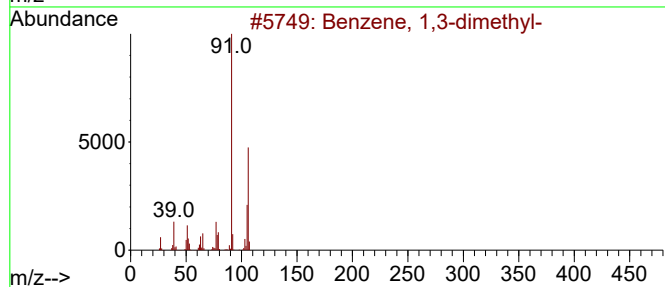
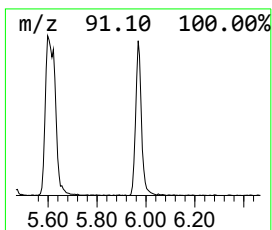
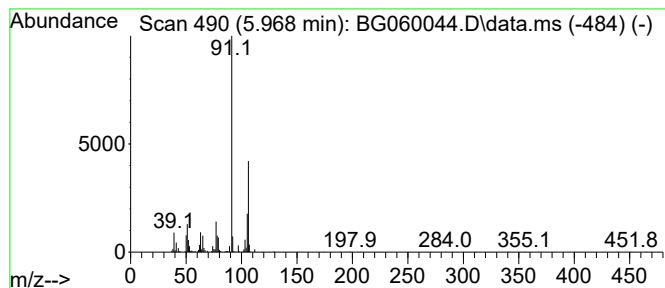
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzene, 1,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.968	32.99 ng	684760	1,4-Dichlorobenzene-d4	7.954

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
2			o-Xylene	106	C8H10	000095-47-6	95
3			p-Xylene	106	C8H10	000106-42-3	95
4			Ethylbenzene	106	C8H10	000100-41-4	87
5			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	87



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ALS Vial : 17 Sample Multiplier: 1

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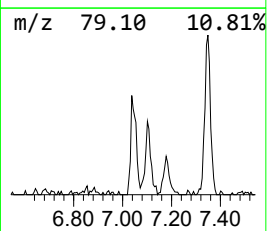
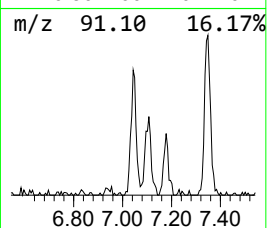
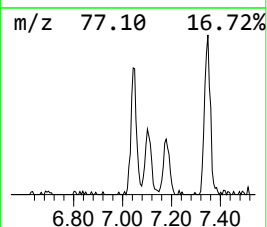
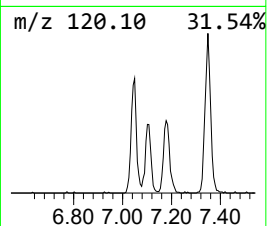
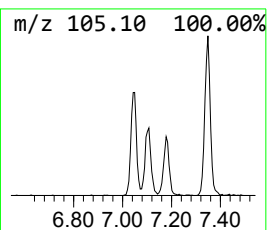
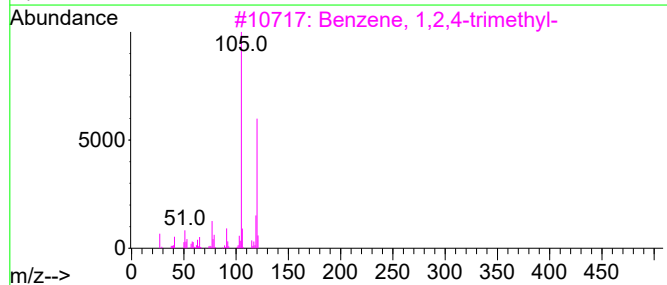
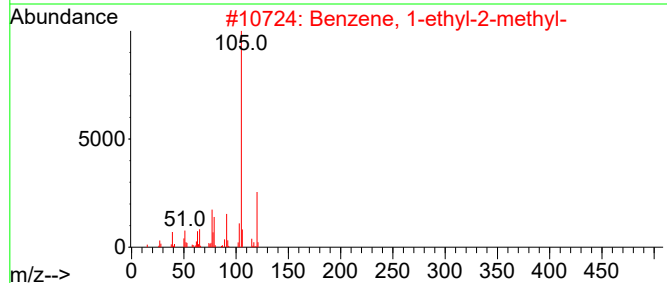
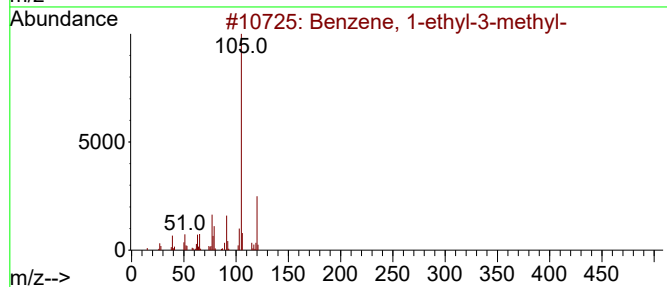
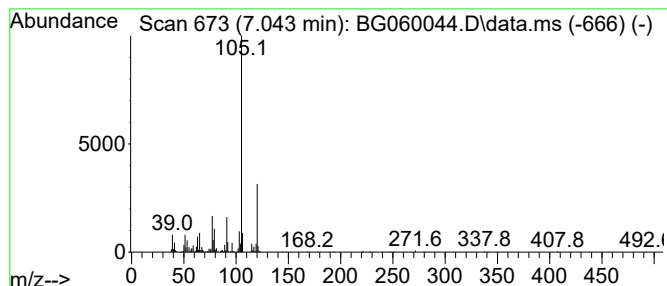
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzene, 1-ethyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.043	16.88 ng	350335	1,4-Dichlorobenzene-d4	7.954

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	87
4			Mesitylene	120	C9H12	000108-67-8	87
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87



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Instrument :
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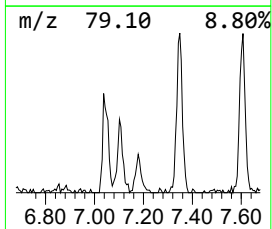
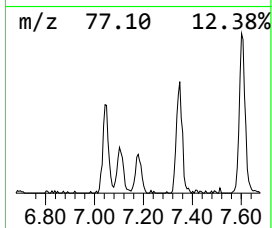
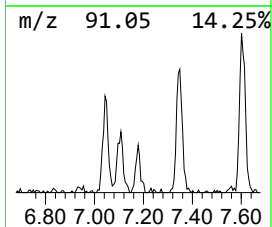
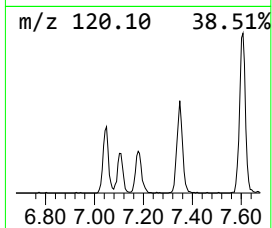
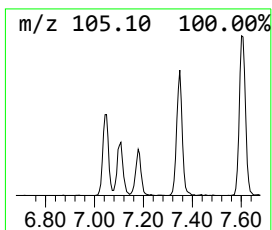
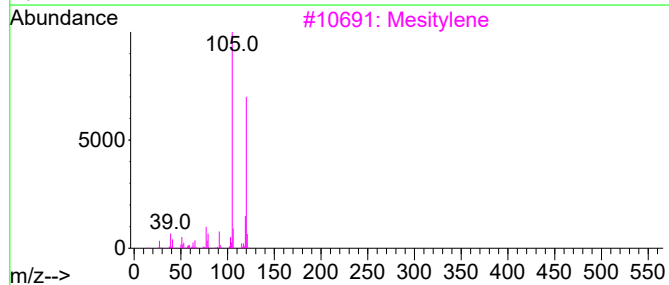
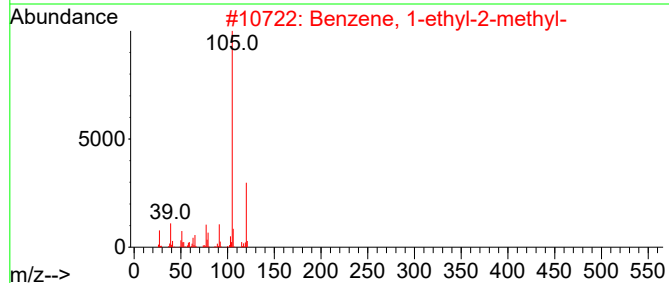
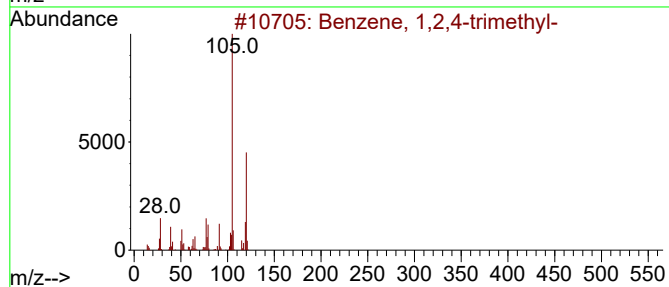
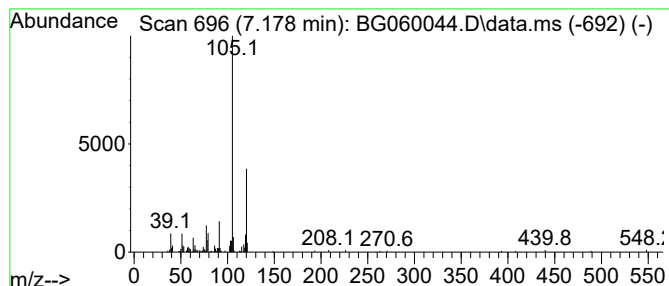
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, 1,2,4-trimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.178	8.94 ng	185508	1,4-Dichlorobenzene-d4	7.954

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	93
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87
3			Mesitylene	120	C9H12	000108-67-8	87
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	81
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	81



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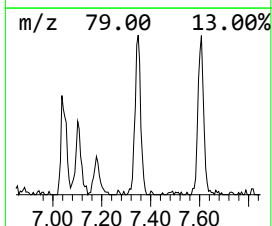
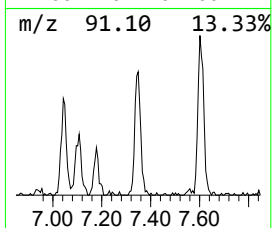
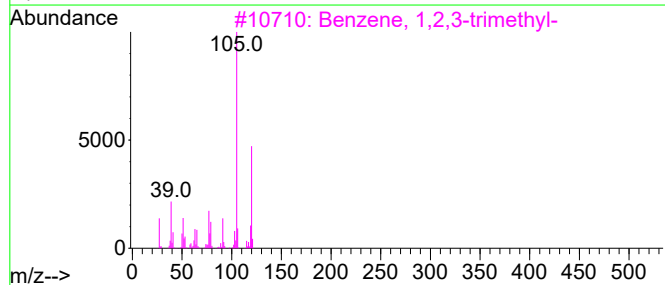
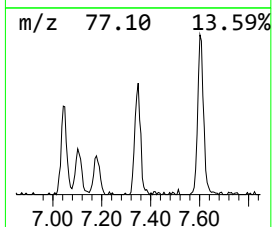
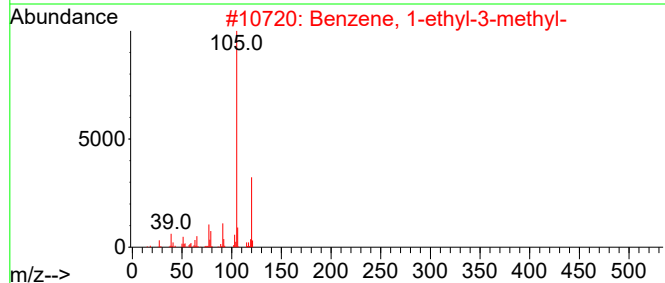
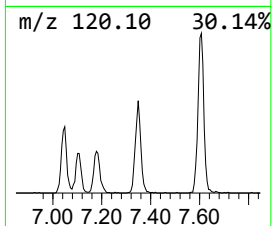
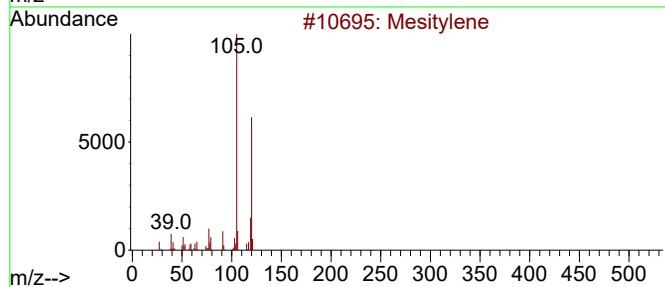
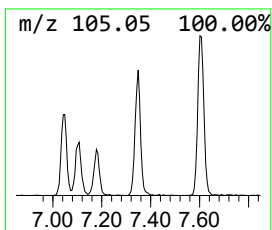
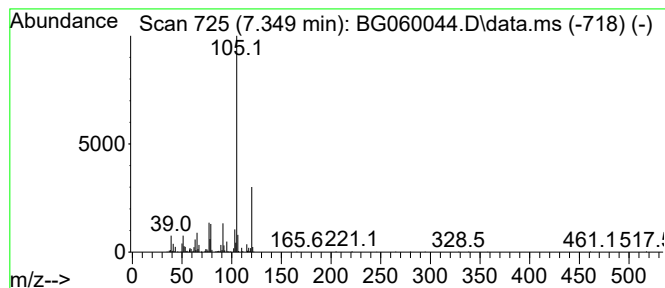
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Mesitylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.349	24.77 ng	514139	1,4-Dichlorobenzene-d4	7.954

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	90
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
Operator : MA/JU
Sample : 05688-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-3

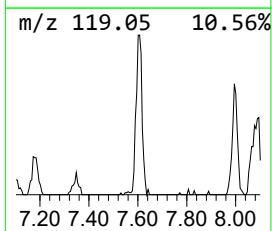
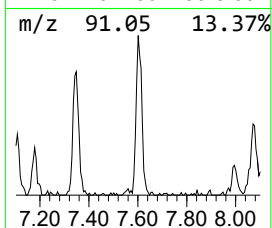
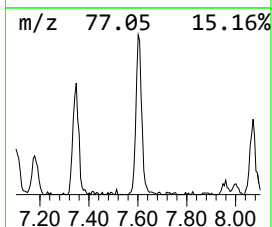
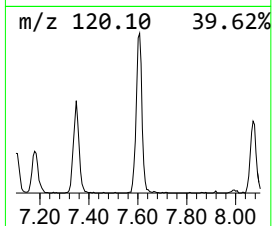
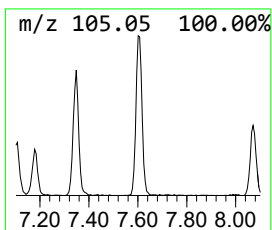
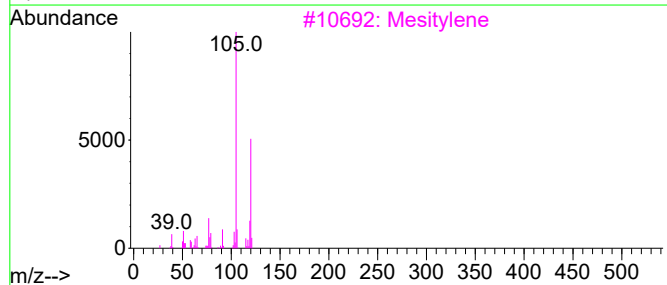
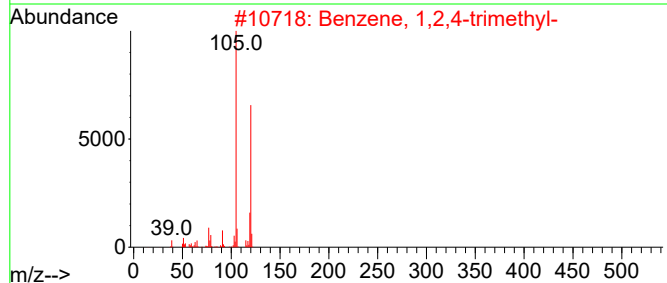
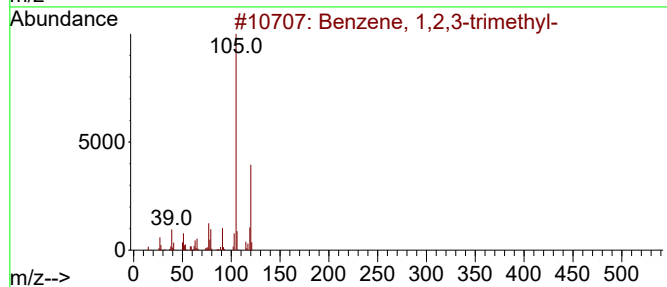
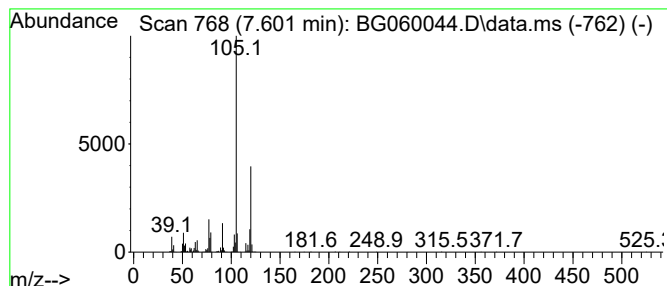
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.601	32.28 ng	669862	1,4-Dichlorobenzene-d4	7.954

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3			Mesitylene	120	C9H12	000108-67-8	94
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
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Sample : 05688-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-3

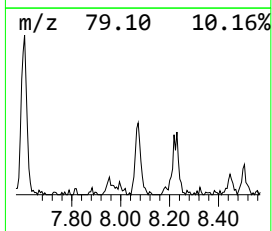
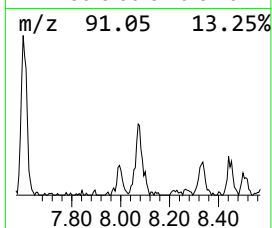
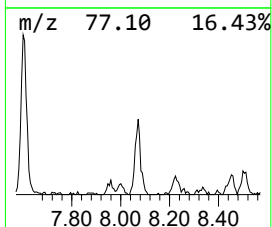
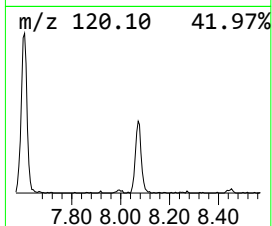
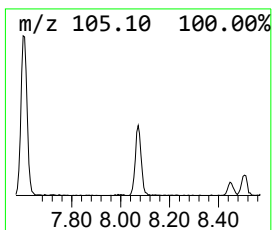
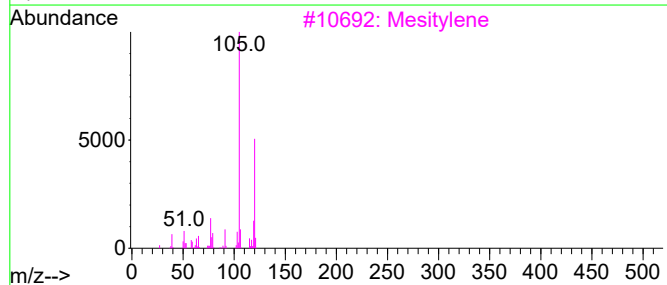
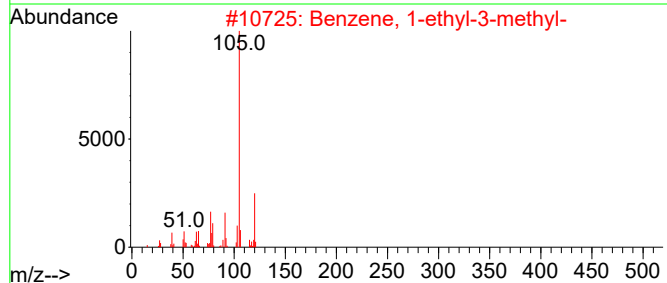
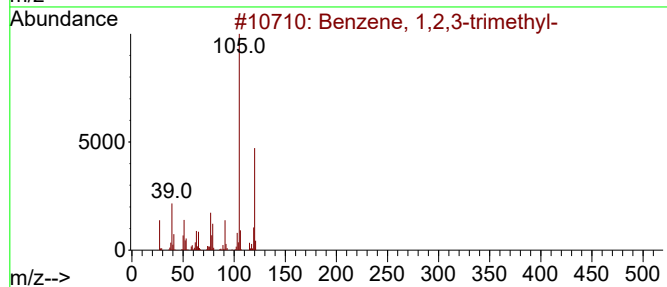
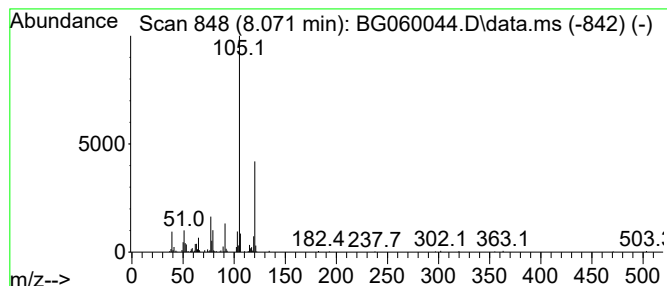
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.071	15.38 ng	319186	1,4-Dichlorobenzene-d4	7.954

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
Operator : MA/JU
Sample : 05688-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

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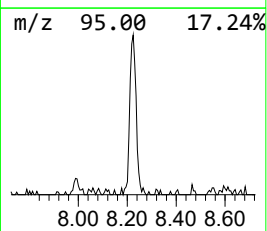
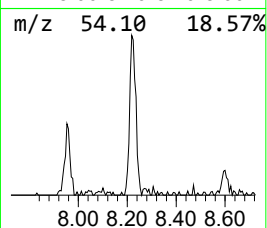
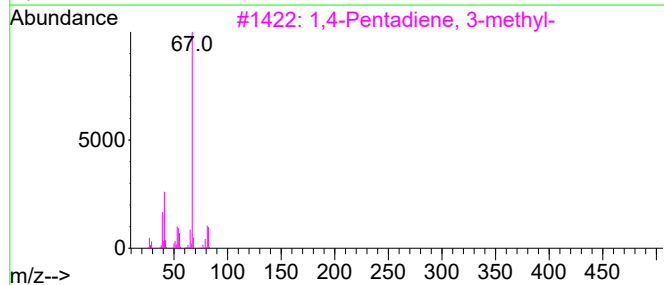
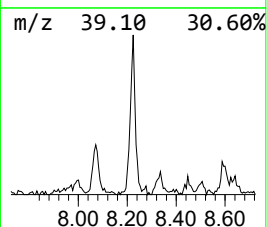
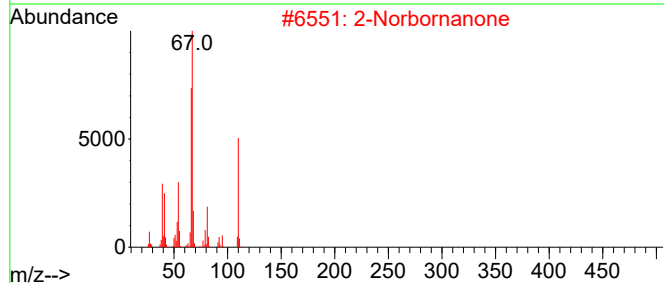
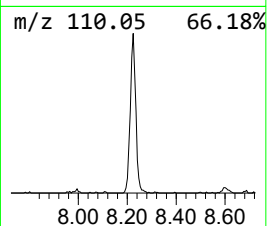
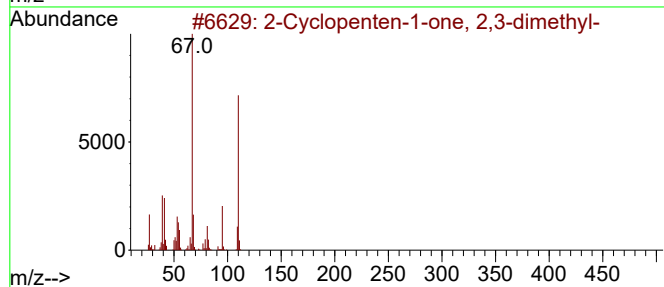
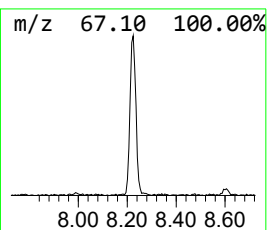
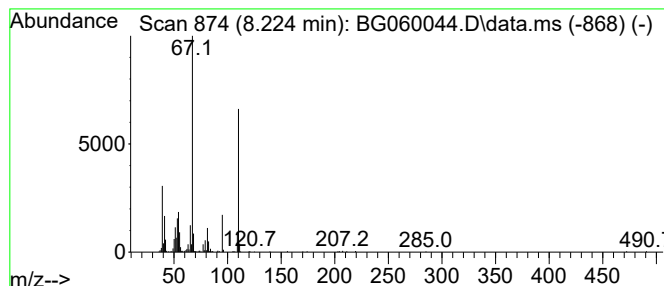
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Cyclopenten-1-one, 2,3-di... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.224	19.23 ng	399185	1,4-Dichlorobenzene-d4	7.954

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Cyclopenten-1-one, 2,3-dimethyl-	110	C7H10O	001121-05-7	91
2		2-Norbornanone	110	C7H10O	000497-38-1	50
3		1,4-Pentadiene, 3-methyl-	82	C6H10	001115-08-8	49
4		1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	47
5		Cyclobutene, 3,3-dimethyl-	82	C6H10	016327-38-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
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Sample : 05688-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

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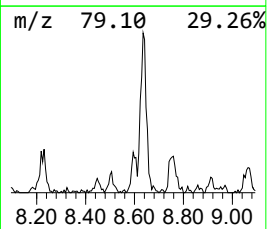
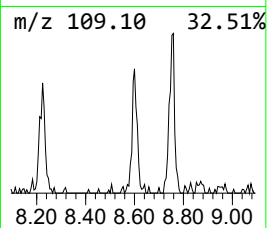
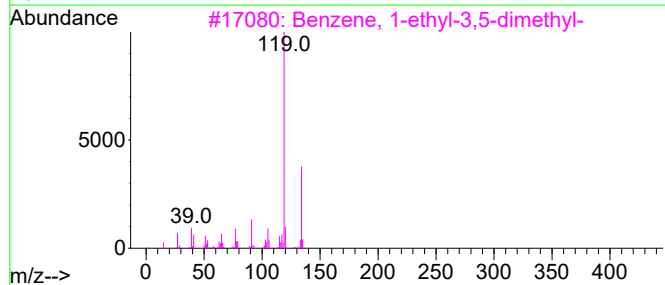
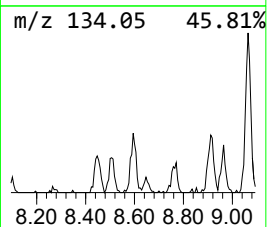
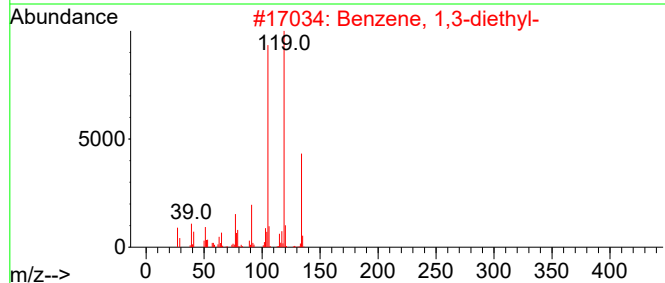
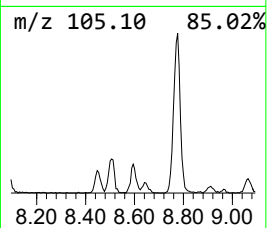
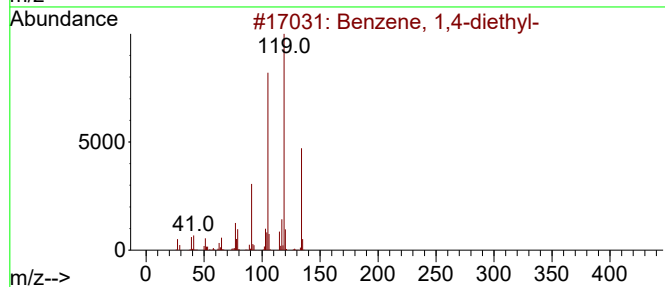
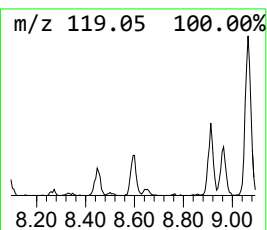
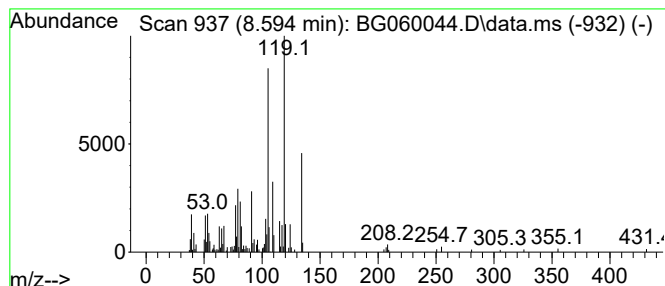
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzene, 1,4-diethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.594	9.42 ng	195469	1,4-Dichlorobenzene-d4	7.954

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	93
2			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	81
3			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	81
4			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	81
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
Operator : MA/JU
Sample : 05688-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-3

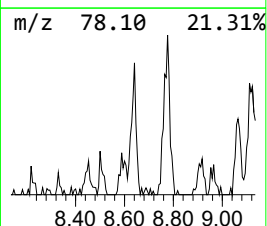
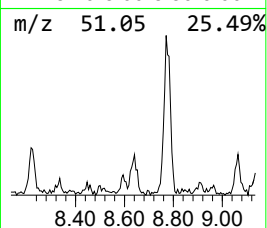
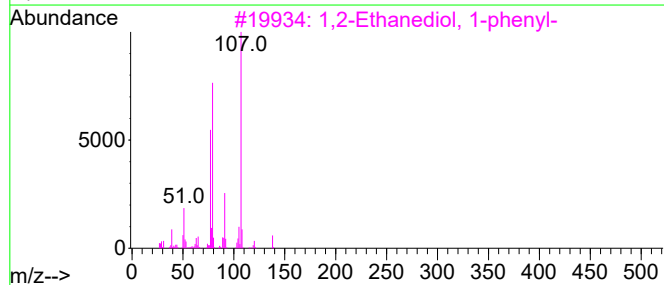
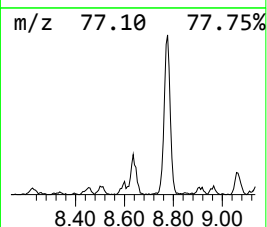
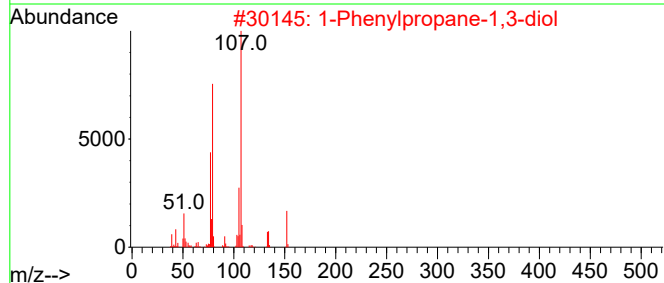
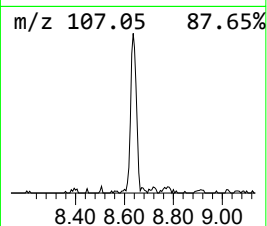
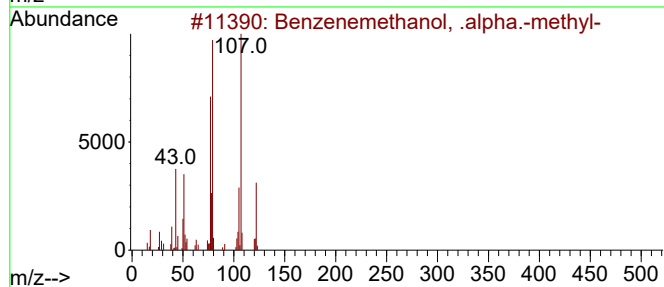
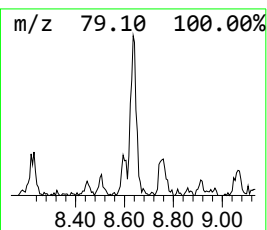
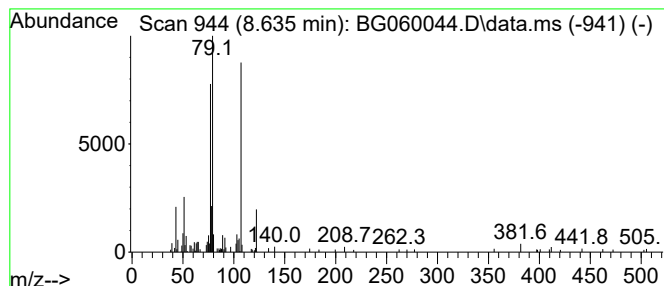
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzenemethanol, .alpha.-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.635	8.00 ng	165983	1,4-Dichlorobenzene-d4	7.954

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenemethanol, .alpha.-methyl-	122	C8H10O	000098-85-1	91
2			1-Phenylpropane-1,3-diol	152	C9H12O2	004850-49-1	72
3			1,2-Ethanediol, 1-phenyl-	138	C8H10O2	000093-56-1	72
4			Benzeneacetic acid, .alpha.-hydr...	152	C8H8O3	017199-29-0	72
5			Mandelamide	151	C8H9NO2	004410-31-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
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Sample : 05688-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

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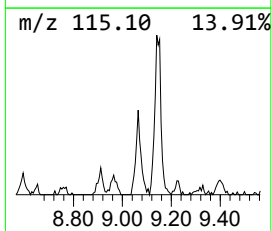
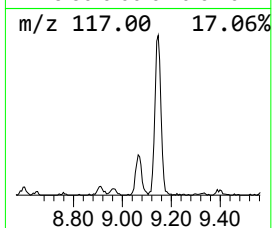
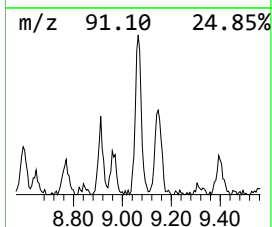
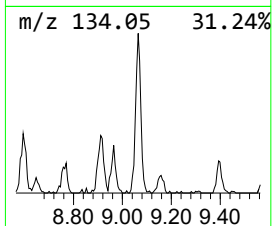
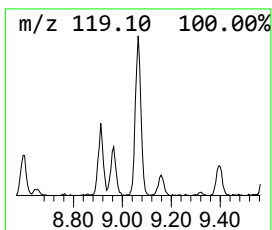
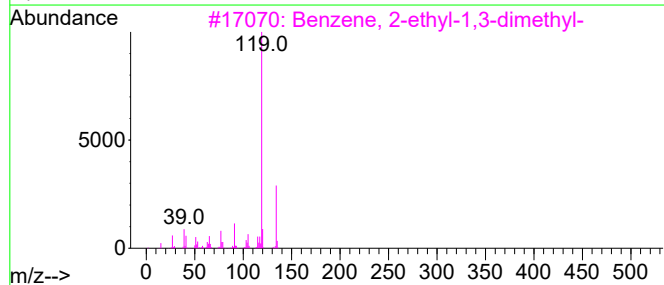
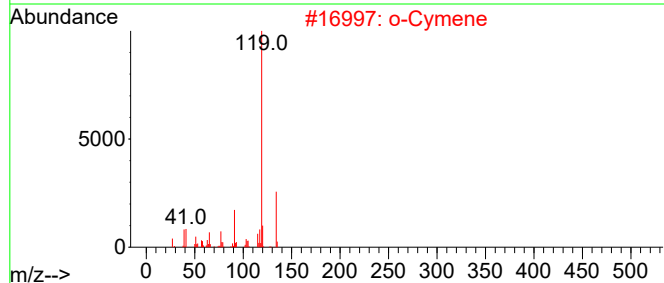
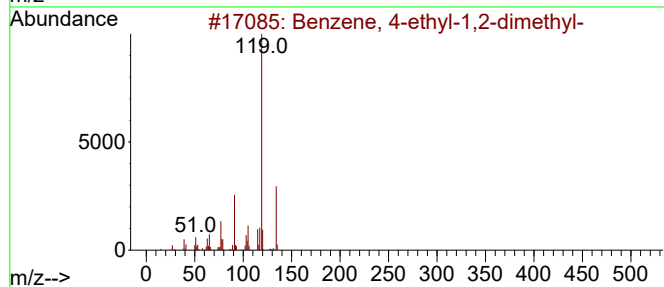
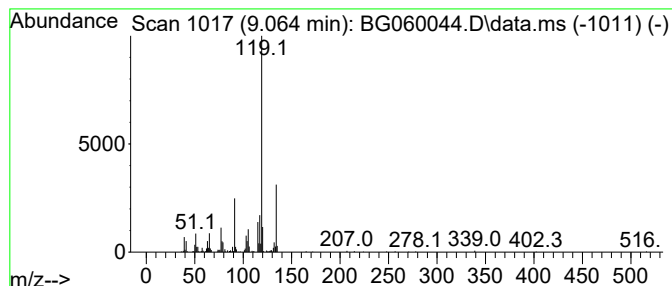
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.064	18.25 ng	378816	1,4-Dichlorobenzene-d4	7.954

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2		o-Cymene	134	C10H14	000527-84-4	94
3		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93
4		p-Cymene	134	C10H14	000099-87-6	93
5		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
Operator : MA/JU
Sample : 05688-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-3

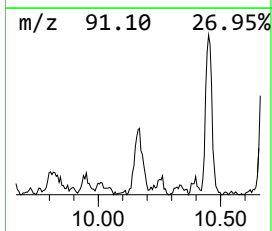
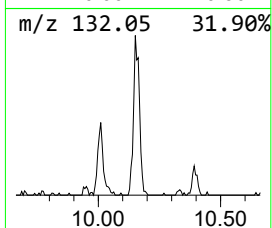
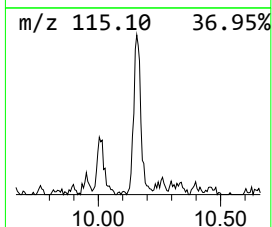
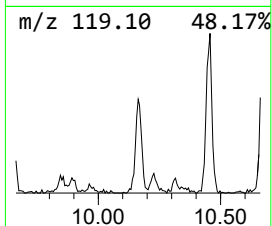
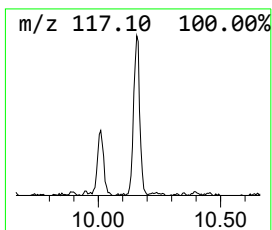
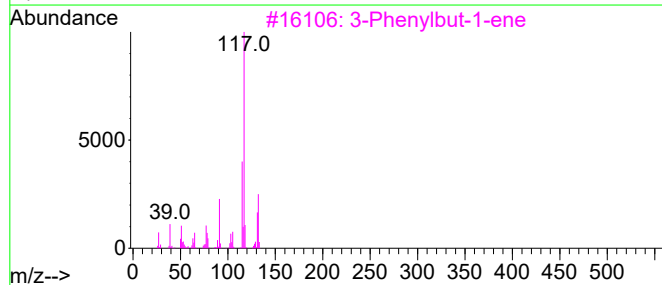
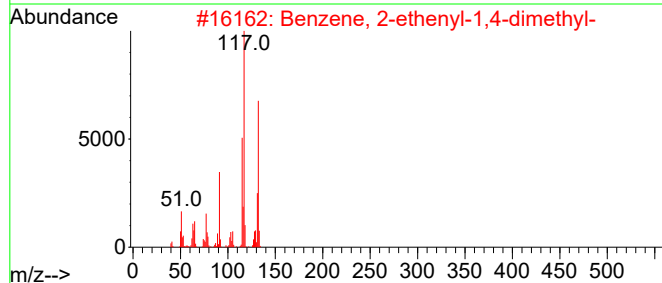
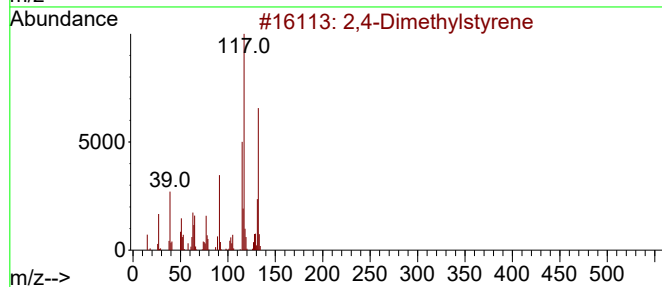
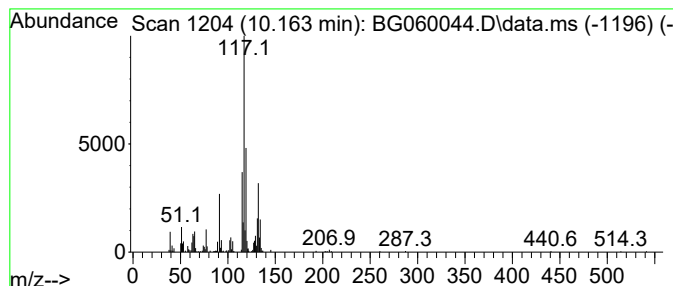
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2,4-Dimethylstyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.163	10.95 ng	388233	Naphthalene-d8	10.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dimethylstyrene	132	C10H12	002234-20-0	70
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	70
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
Operator : MA/JU
Sample : 05688-04
Misc :
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Instrument :
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ClientSampleId :
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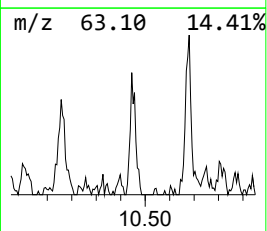
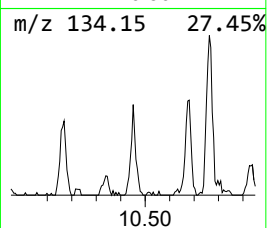
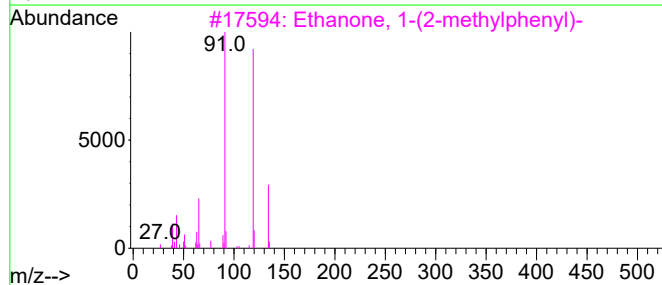
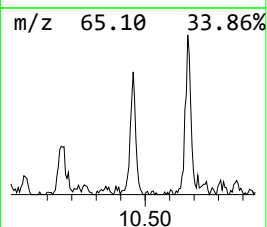
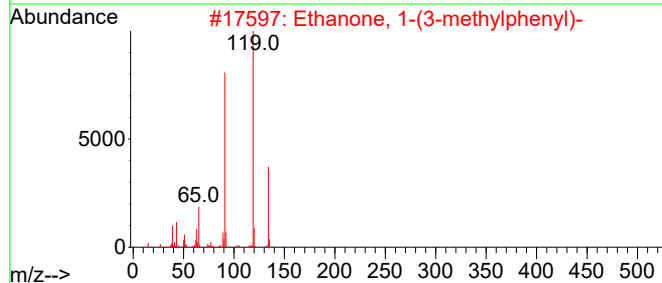
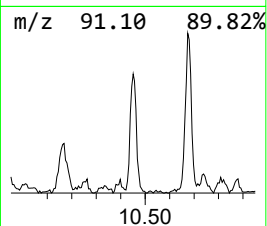
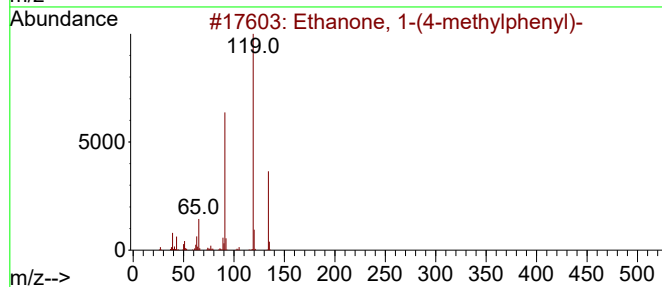
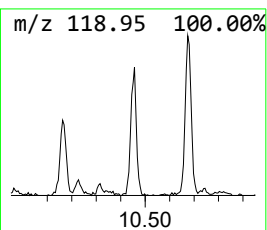
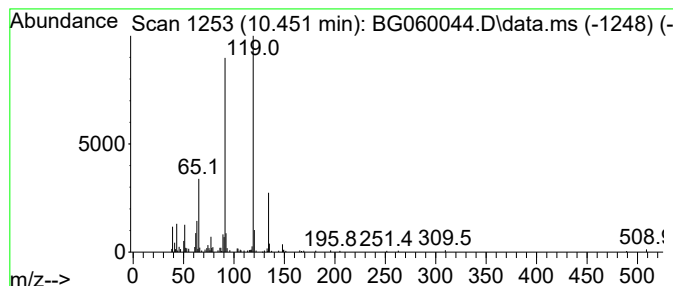
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Ethanone, 1-(4-methylphenyl)- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.451	6.37 ng	225824	Naphthalene-d8	10.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	94
2			Ethanone, 1-(3-methylphenyl)-	134	C9H10O	000585-74-0	94
3			Ethanone, 1-(2-methylphenyl)-	134	C9H10O	000577-16-2	91
4			Propiophenone, 2'-methyl-	148	C10H12O	002040-14-4	74
5			N-Methyl-p-toluamide	149	C9H11NO	018370-11-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
Operator : MA/JU
Sample : 05688-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-3

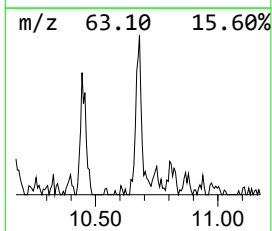
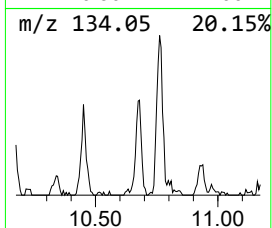
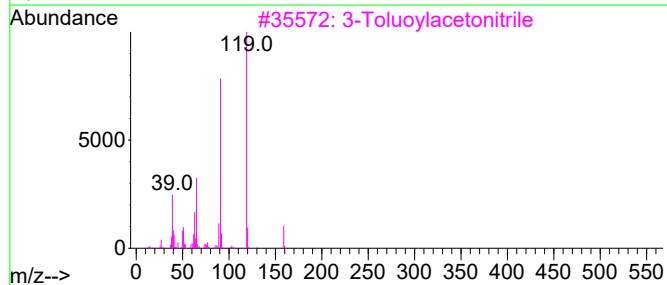
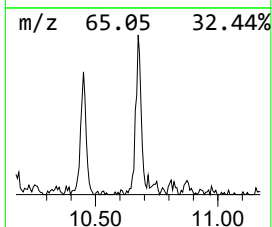
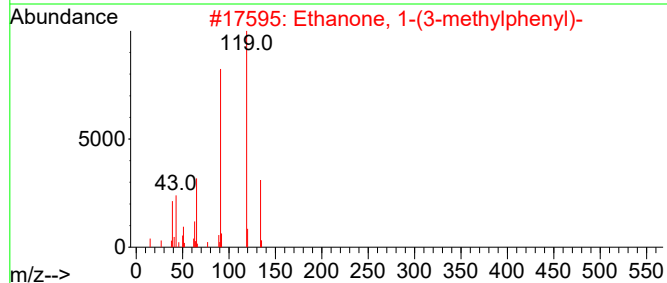
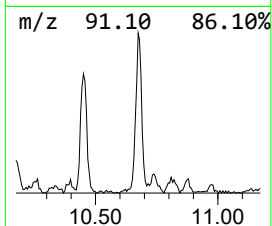
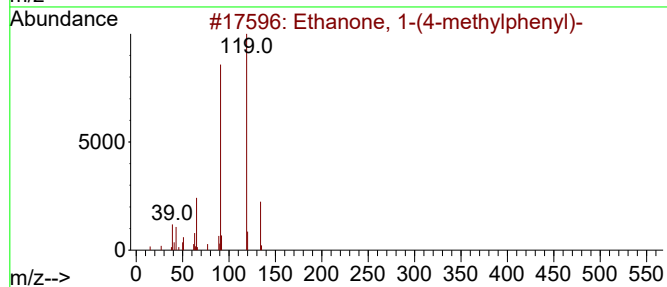
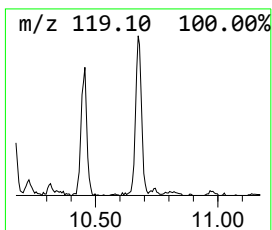
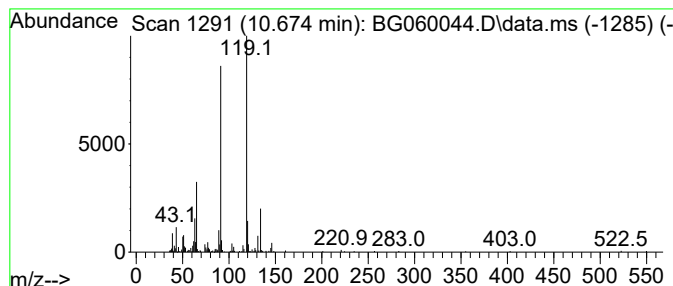
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Ethanone, 1-(3-methylphenyl)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.674	7.95 ng	281845	Naphthalene-d8	10.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	90
2			Ethanone, 1-(3-methylphenyl)-	134	C9H10O	000585-74-0	87
3			3-Toluoylacetonitrile	159	C10H9NO	053882-81-8	72
4			4-(Trifluoroacetyl)toluene	188	C9H7F3O	1000342-44-2	64
5			4-Methylbenzoyl isothiocyanate	177	C9H7NOS	016794-68-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
Operator : MA/JU
Sample : 05688-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

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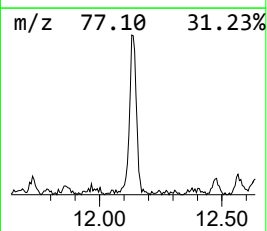
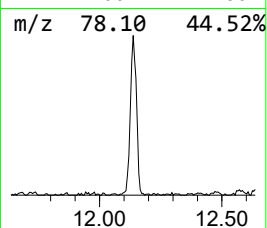
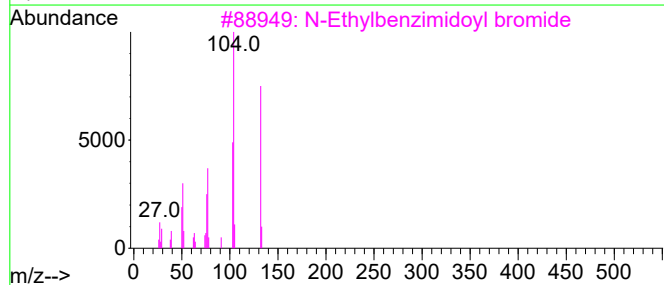
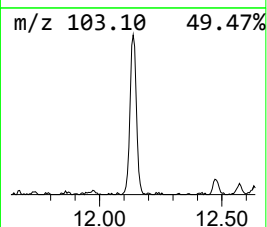
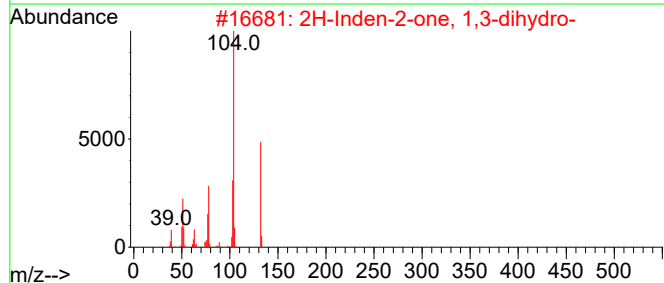
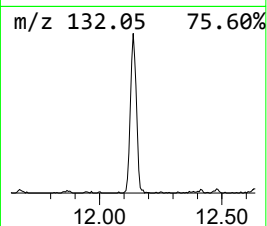
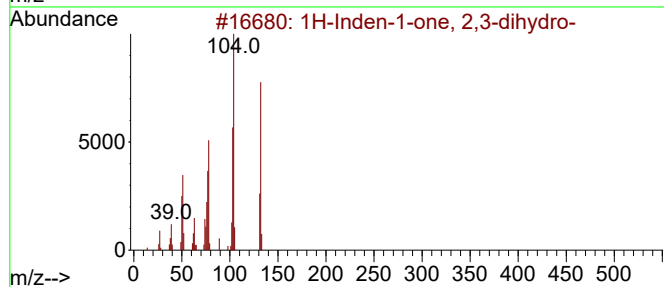
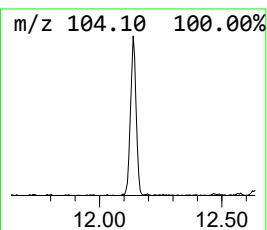
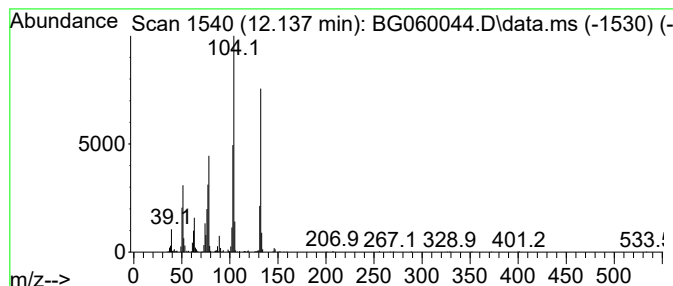
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.137	21.24 ng	752745	Naphthalene-d8	10.762

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	98
2		2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	60
3		N-Ethylbenzimidoyl bromide	211	C9H10BrN	041182-87-0	58
4		Styrene	104	C8H8	000100-42-5	55
5		1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
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Sample : 05688-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

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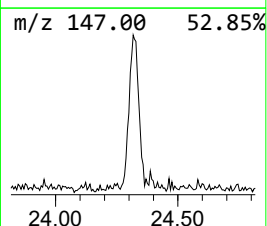
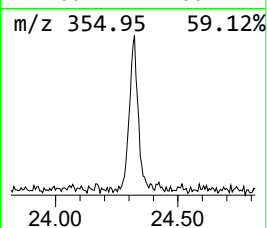
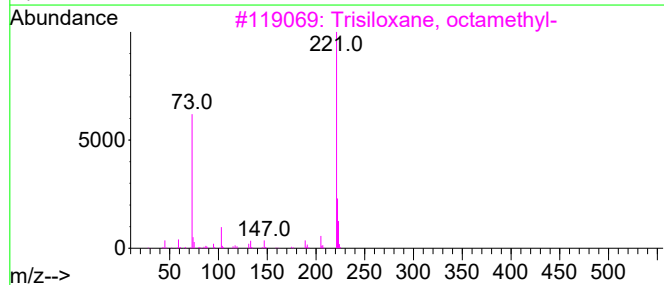
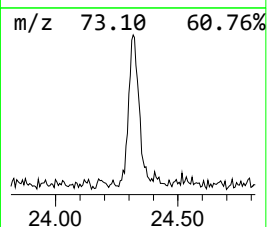
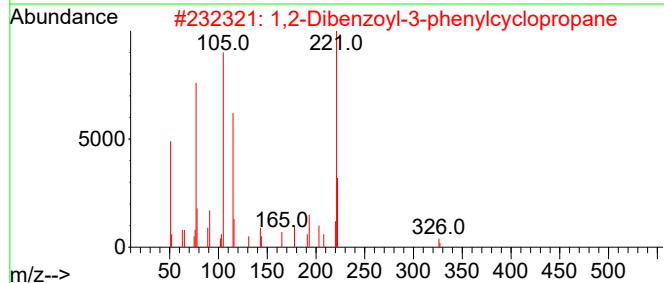
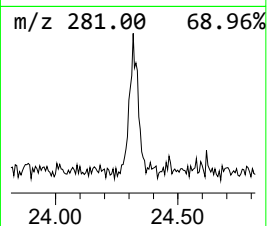
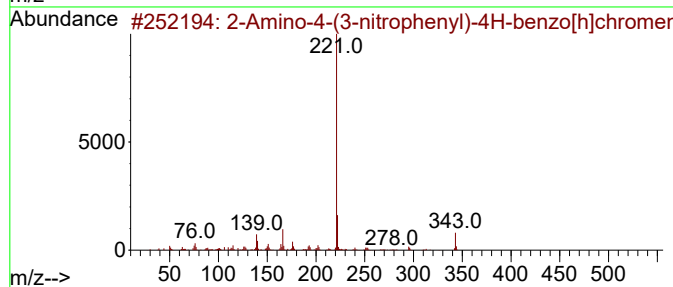
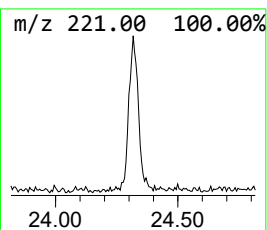
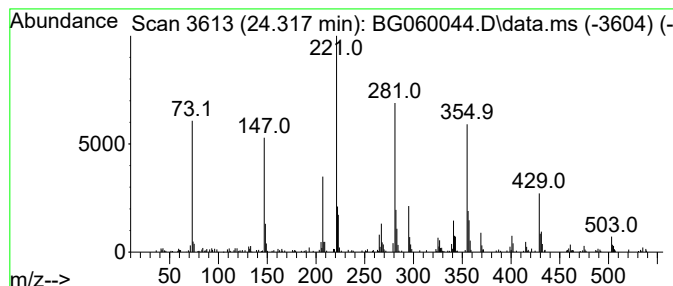
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown24.317 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.317	6.04 ng	653737	Perylene-d12	24.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Amino-4-(3-nitrophenyl)-4H-ben...	343	C20H13N3O3	149550-36-7	27
2			1,2-Dibenzoyl-3-phenylcyclopropane	326	C23H18O2	029128-64-1	25
3			Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	22
4			1,3,5-Trisiloxane, 1,1,3,3,5,5-h...	320	C14H36O2Si3	1000458-50-5	22
5			3-Oxobutan-2-yl trimethylsilyl p...	308	C15H20O5Si	1000373-49-5	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
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Sample : 05688-04
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ClientSampleId :
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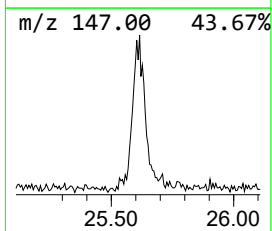
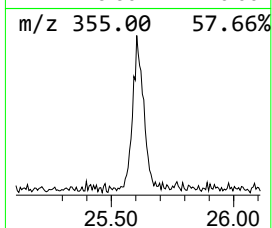
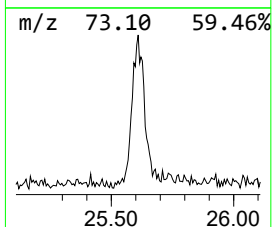
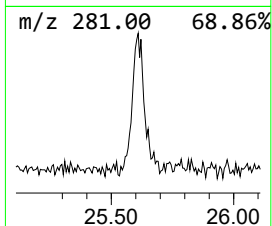
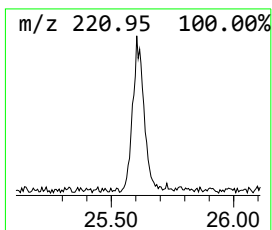
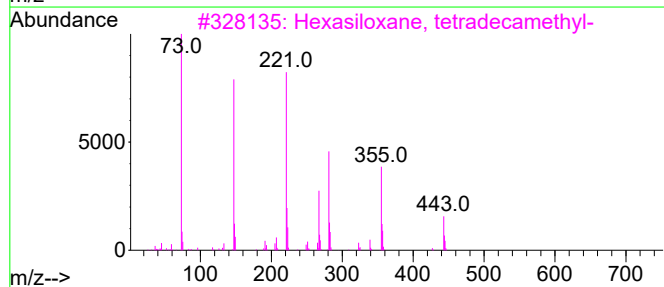
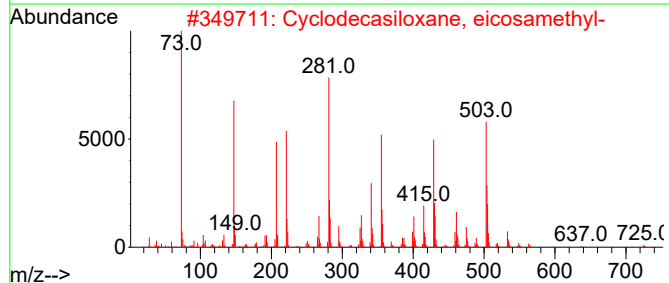
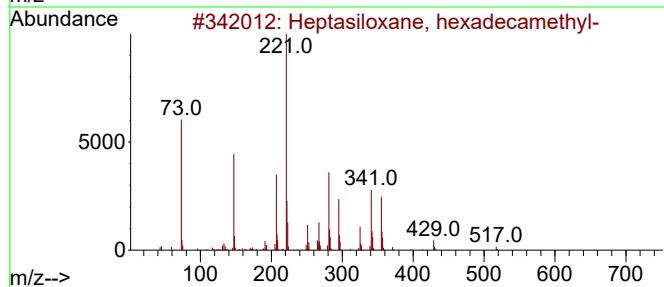
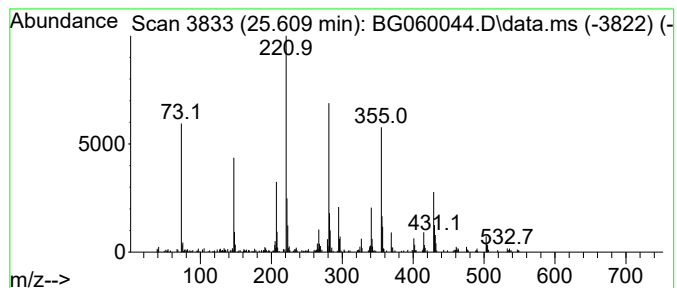
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown25.610 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.610	7.19 ng	777578	Perylene-d12	24.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	49
2			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	46
3			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	38
4			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	25
5			Isophthalic acid, bis(methoxycar...	310	C14H14O8	1010162-18-4	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
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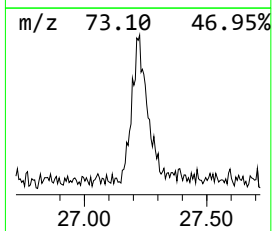
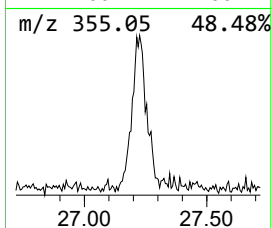
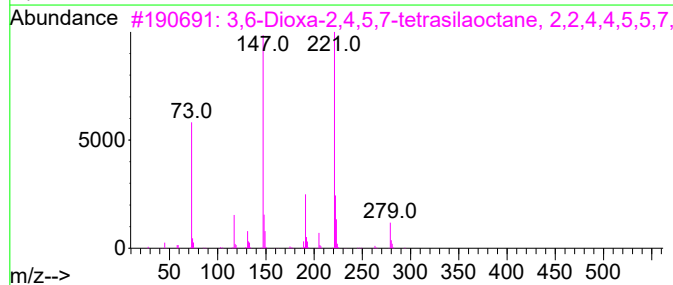
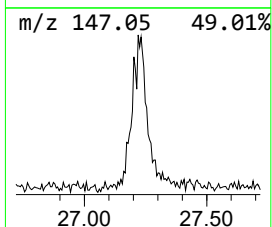
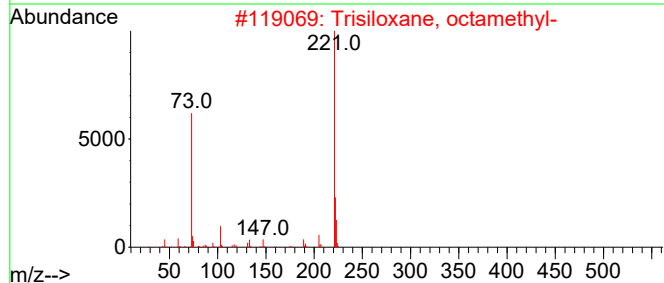
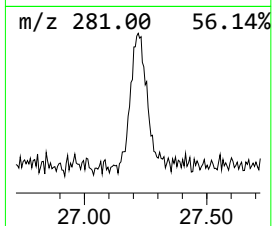
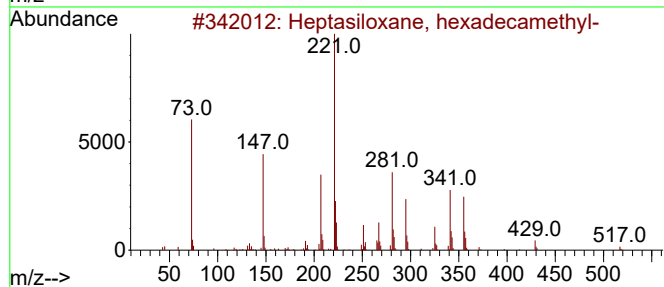
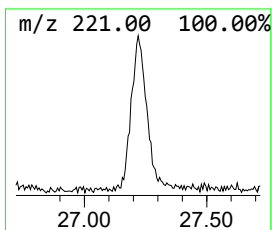
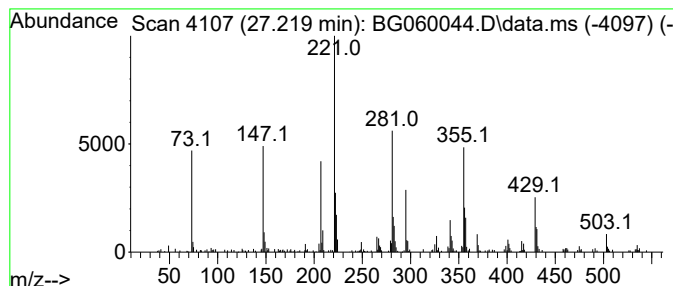
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown27.219 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.219	7.07 ng	764916	Perylene-d12	24.799

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
2		Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	14
3		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	10
4		2'-Hydroxychalcone, O-trimethyls...	296	C18H20O2Si	1000451-93-1	10
5		benzenamine, N-[bis(2,4,6-trimet...	341	C24H28BN	1000398-20-2	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060044.D
Acq On : 15 Dec 2023 20:34
Operator : MA/JU
Sample : 05688-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-3

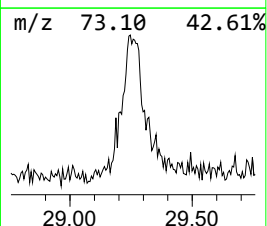
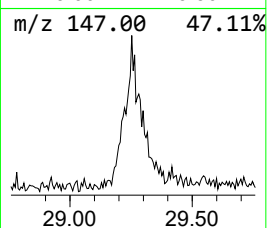
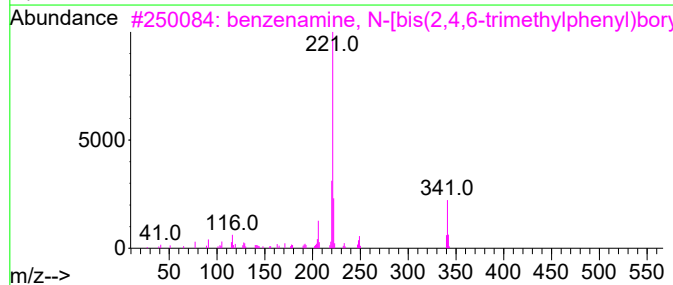
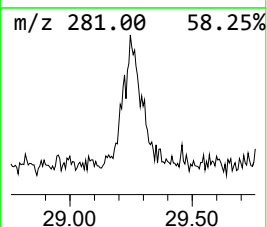
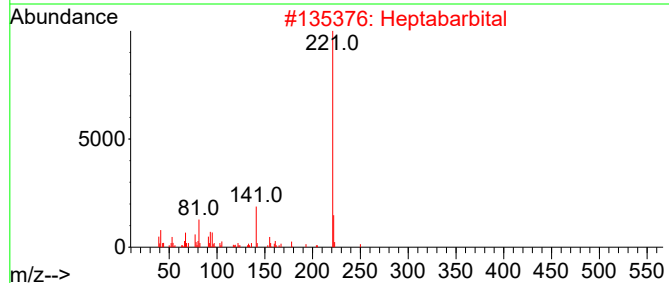
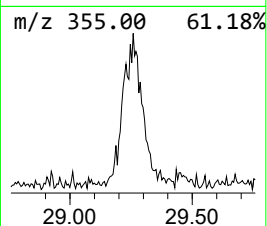
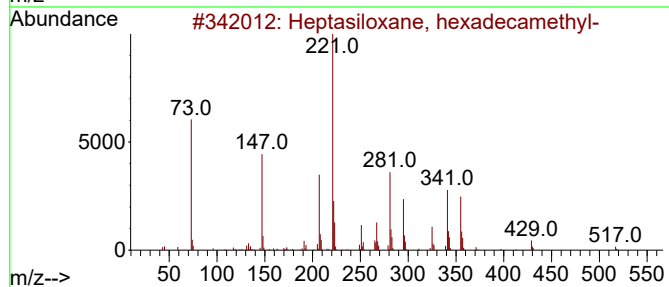
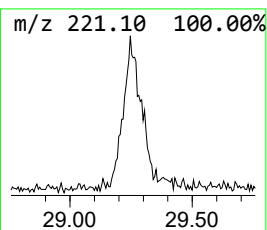
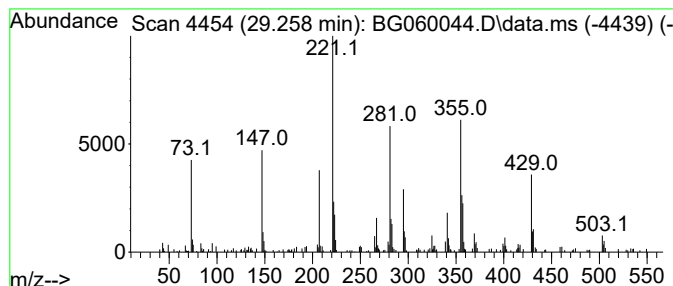
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown29.258 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.258	7.13 ng	771015	Perylene-d12	24.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	46
2			Heptabarbital	250	C13H18N2O3	000509-86-4	22
3			benzenamine, N-[bis(2,4,6-trimet...	341	C24H28BN	1000398-20-2	22
4			Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	22
5			Indole, 3-benzoyl-	221	C15H11NO	015224-25-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
 Data File : BG060044.D
 Acq On : 15 Dec 2023 20:34
 Operator : MA/JU
 Sample : 05688-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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...	3.142	52.8	ng	1095650	1	7.954	415085	20.0
Benzene, 1,3-di...	5.968	33.0	ng	684760	1	7.954	415085	20.0
Benzene, 1-ethy...	7.043	16.9	ng	350335	1	7.954	415085	20.0
Benzene, 1,2,4-...	7.178	8.9	ng	185508	1	7.954	415085	20.0
Mesitylene	7.349	24.8	ng	514139	1	7.954	415085	20.0
Benzene, 1,2,3-...	7.601	32.3	ng	669862	1	7.954	415085	20.0
Benzene, 1-ethy...	8.071	15.4	ng	319186	1	7.954	415085	20.0
2-Cyclopenten-1...	8.224	19.2	ng	399185	1	7.954	415085	20.0
Benzene, 1,4-di...	8.594	9.4	ng	195469	1	7.954	415085	20.0
Benzenemethanol...	8.635	8.0	ng	165983	1	7.954	415085	20.0
Benzene, 4-ethy...	9.064	18.3	ng	378816	1	7.954	415085	20.0
2,4-Dimethylsty...	10.163	10.9	ng	388233	2	10.762	708830	20.0
Ethanone, 1-(4-...	10.451	6.4	ng	225824	2	10.762	708830	20.0
Ethanone, 1-(3-...	10.674	8.0	ng	281845	2	10.762	708830	20.0
1H-Inden-1-one,...	12.137	21.2	ng	752745	2	10.762	708830	20.0
unknown24.317	24.317	6.0	ng	653737	6	24.799	2163970	20.0
unknown25.610	25.610	7.2	ng	777578	6	24.799	2163970	20.0
unknown27.219	27.219	7.1	ng	764916	6	24.799	2163970	20.0
unknown29.258	29.258	7.1	ng	771015	6	24.799	2163970	20.0