

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
 Data File : BG053556.D
 Acq On : 13 May 2022 23:39
 Operator : CG/JU
 Sample : N2829-01 5X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 OK-02-051222

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-BG050522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053556.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.535	21	25	30	rVB	10126	14980	1.68%	0.098%
2	3.853	74	79	85	rBV	16083	28929	3.25%	0.189%
3	3.947	91	95	103	rBV	21234	39190	4.40%	0.256%
4	5.656	380	386	395	rBV	67512	118557	13.31%	0.774%
5	7.254	647	658	671	rBV4	84235	298843	33.56%	1.951%
6	7.407	678	684	693	rBV2	36745	68592	7.70%	0.448%
7	7.495	693	699	708	rVB	34269	59259	6.65%	0.387%
8	7.653	719	726	734	rBV2	49802	85708	9.62%	0.560%
9	7.976	775	781	788	rBV	58225	98005	11.01%	0.640%
10	8.082	792	799	803	rBV	143222	258378	29.01%	1.687%
11	8.323	834	840	852	rBV2	56902	105634	11.86%	0.690%
12	8.440	852	860	867	rVB2	56301	99086	11.13%	0.647%
13	8.529	867	875	882	rBV	67522	118193	13.27%	0.772%
14	8.605	882	888	896	rVB2	33963	80939	9.09%	0.528%
15	8.887	925	936	937	rBV3	75687	206872	23.23%	1.351%
16	9.175	978	985	991	rBV	49300	84235	9.46%	0.550%
17	9.245	991	997	1001	rBV	51935	92297	10.36%	0.603%
18	9.286	1001	1004	1013	rVB	44796	82617	9.28%	0.539%
19	9.492	1033	1039	1047	rBV3	17015	28408	3.19%	0.185%
20	9.809	1085	1093	1100	rBV	70078	118714	13.33%	0.775%
21	10.009	1120	1127	1131	rBV2	39761	74246	8.34%	0.485%
22	10.062	1131	1136	1145	rVB	75318	129192	14.51%	0.844%
23	10.220	1156	1163	1164	rBV2	7154	13922	1.56%	0.091%
24	10.291	1169	1175	1182	rVB	48818	86136	9.67%	0.562%
25	10.549	1213	1219	1228	rBV3	56712	108417	12.17%	0.708%
26	10.755	1248	1254	1263	rVB	68535	122209	13.72%	0.798%
27	10.896	1271	1278	1283	rBV	191736	355909	39.97%	2.324%
28	10.943	1283	1286	1295	rVB	81537	140762	15.81%	0.919%
29	11.055	1295	1305	1312	rBV2	35271	70851	7.96%	0.463%
30	11.231	1328	1335	1341	rVB	80796	130268	14.63%	0.851%
31	11.801	1425	1432	1443	rBV	33482	70378	7.90%	0.460%
32	12.177	1488	1496	1507	rBV	69752	118942	13.36%	0.777%
33	12.423	1532	1538	1545	rVB	23668	37346	4.19%	0.244%
34	12.541	1552	1558	1569	rVB	97880	172007	19.32%	1.123%
35	12.676	1575	1581	1588	rBV2	23655	45988	5.16%	0.300%
36	12.764	1588	1596	1603	rVB	102376	178574	20.05%	1.166%

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37	12.911	1613	1621	1629	rVB3	96251	189412	21.27%	1.237%
38	13.152	1657	1662	1667	rBV2	76414	122831	13.79%	0.802%
39	13.234	1671	1676	1686	rVV2	65931	117877	13.24%	0.770%
40	13.328	1686	1692	1700	rVB	130971	206473	23.19%	1.348%
41	13.545	1722	1729	1733	rBV	125458	207442	23.29%	1.354%
42	13.586	1733	1736	1745	rVB	100145	158863	17.84%	1.037%
43	13.792	1761	1771	1778	rBV2	54592	98529	11.06%	0.643%
44	14.074	1814	1819	1826	rBV2	41947	67309	7.56%	0.439%
45	14.156	1826	1833	1839	rVV	98747	151055	16.96%	0.986%
46	14.221	1839	1844	1849	rVV	48036	76509	8.59%	0.500%
47	14.274	1849	1853	1860	rVB3	67942	108138	12.14%	0.706%
48	14.379	1864	1871	1875	rBV2	42454	65383	7.34%	0.427%
49	14.432	1875	1880	1886	rVB	114785	180018	20.22%	1.175%
50	14.614	1903	1911	1919	rBV	43865	80323	9.02%	0.524%
51	14.708	1919	1927	1933	rVV	307019	482237	54.15%	3.149%
52	14.773	1933	1938	1944	rVV	138136	203266	22.83%	1.327%
53	14.832	1944	1948	1957	rVV3	17451	36816	4.13%	0.240%
54	14.938	1960	1966	1973	rVV	61647	128359	14.41%	0.838%
55	14.990	1973	1975	1982	rVV4	17217	31824	3.57%	0.208%
56	15.067	1984	1988	1991	rVV	69326	105850	11.89%	0.691%
57	15.108	1991	1995	2005	rVB	118039	194404	21.83%	1.269%
58	15.255	2014	2020	2028	rBV	65024	109405	12.29%	0.714%
59	15.337	2028	2034	2044	rVB2	71079	121449	13.64%	0.793%
60	15.513	2058	2064	2070	rBV	113985	167915	18.86%	1.096%
61	15.748	2097	2104	2115	rBV3	213020	473555	53.18%	3.092%
62	15.836	2115	2119	2124	rVB3	21936	35132	3.95%	0.229%
63	15.954	2134	2139	2146	rBV	143532	206169	23.15%	1.346%
64	16.036	2146	2153	2161	rVB	105882	163790	18.39%	1.069%
65	16.195	2171	2180	2188	rBV	91157	148691	16.70%	0.971%
66	16.635	2248	2255	2260	rBV	111514	161561	18.14%	1.055%
67	16.764	2270	2277	2283	rBV	109971	168999	18.98%	1.103%
68	16.900	2293	2300	2305	rBV	109065	157219	17.66%	1.027%
69	17.117	2331	2337	2345	rBV2	91539	164114	18.43%	1.072%
70	17.458	2388	2395	2398	rBV	354325	546761	61.40%	3.570%
71	17.499	2398	2402	2409	rVB	200575	293487	32.96%	1.916%
72	17.587	2411	2417	2424	rBV	153097	241356	27.10%	1.576%
73	17.857	2458	2463	2469	rVV	133600	205359	23.06%	1.341%
74	18.333	2538	2544	2549	rBV4	16612	29545	3.32%	0.193%
75	18.403	2549	2556	2561	rVV	150978	212776	23.89%	1.389%
76	18.527	2572	2577	2581	rVV3	18356	34443	3.87%	0.225%

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77	18.562	2581	2583	2588	rVV3	8453	11471	1.29%	0.075%
78	18.962	2646	2651	2657	rBV8	10254	17834	2.00%	0.116%
79	19.243	2693	2699	2703	rBV3	18013	32762	3.68%	0.214%
80	19.502	2738	2743	2750	rBV	245598	363515	40.82%	2.373%
81	19.684	2770	2774	2780	rVB	20617	36706	4.12%	0.240%
82	19.866	2795	2805	2812	rBV	252399	397202	44.60%	2.593%
83	20.054	2832	2837	2842	rVB	212605	274787	30.86%	1.794%
84	20.354	2885	2888	2893	rVB3	27139	32119	3.61%	0.210%
85	20.741	2949	2954	2959	rVB	146387	196680	22.09%	1.284%
86	20.806	2960	2965	2969	rVB	178406	209054	23.48%	1.365%
87	21.358	3055	3059	3064	rBV5	23436	34293	3.85%	0.224%
88	21.605	3096	3101	3110	rBV2	172971	332912	37.38%	2.174%
89	21.734	3114	3123	3128	rVV2	377972	890502	100.00%	5.814%
90	21.781	3128	3131	3142	rVB	180409	276984	31.10%	1.809%
91	22.827	3304	3309	3315	rVB	122889	215053	24.15%	1.404%
92	23.972	3497	3504	3509	rBV	103613	257833	28.95%	1.683%
93	24.037	3510	3515	3522	rVB	116284	267723	30.06%	1.748%
94	24.859	3647	3655	3666	rVB	103632	290704	32.64%	1.898%
95	25.018	3673	3682	3693	rVB	198749	580267	65.16%	3.789%

Sum of corrected areas: 15315628

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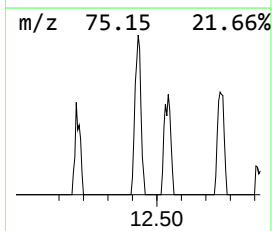
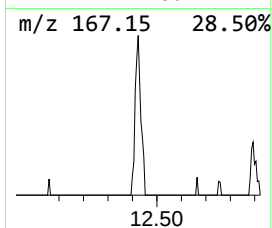
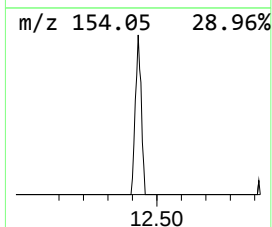
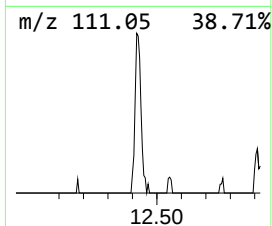
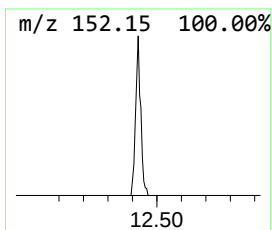
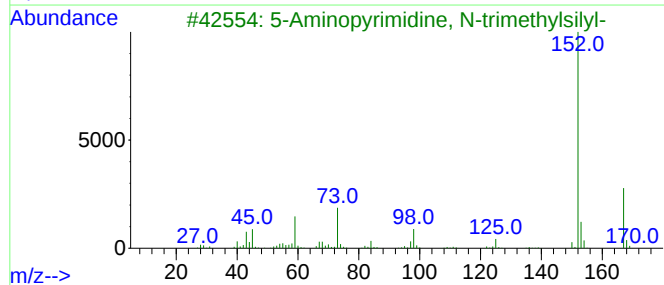
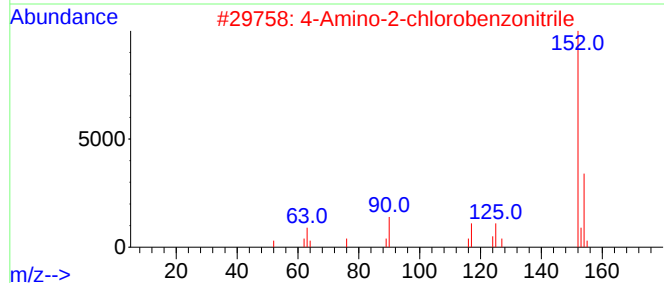
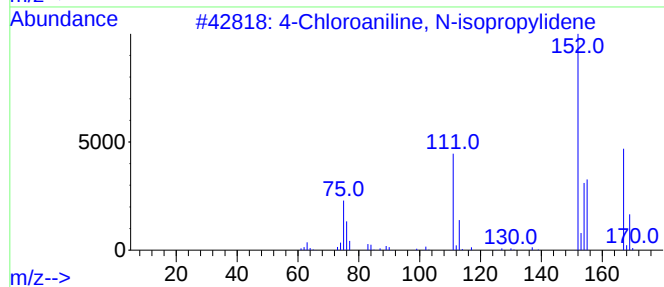
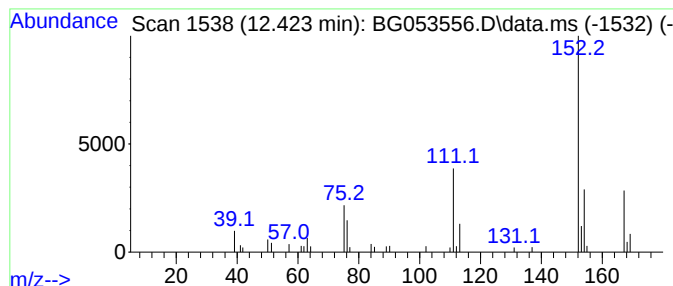
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Chloroaniline, N-isopropy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.423	2.10 ng	37346	Naphthalene-d8	10.896

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Chloroaniline, N-isopropylidene	167	C9H10ClN	040938-43-0	53
2			4-Amino-2-chlorobenzonitrile	152	C7H5ClN2	020925-27-3	43
3			5-Aminopyrimidine, N-trimethylsi...	167	C7H13N3Si	1000493-88-4	38
4			3-Chloro-1H-indazole	152	C7H5ClN2	029110-74-5	38
5			5-Chlorobenzimidazole	152	C7H5ClN2	004887-82-5	38



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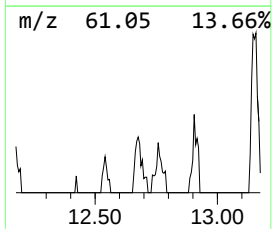
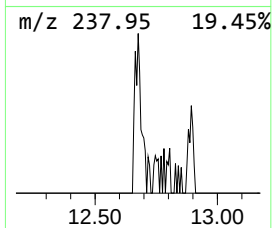
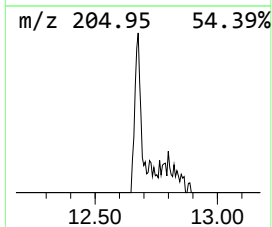
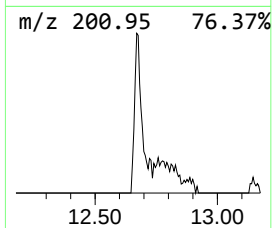
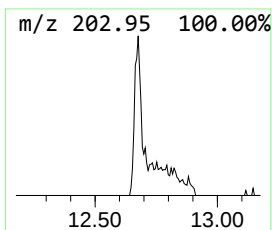
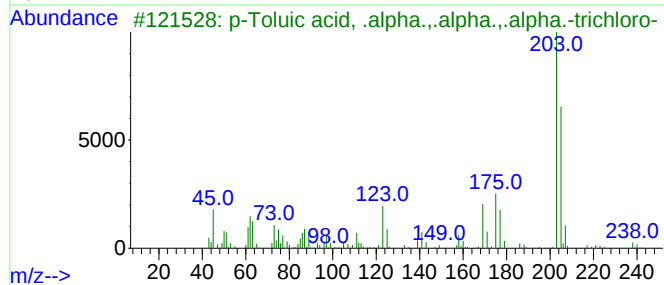
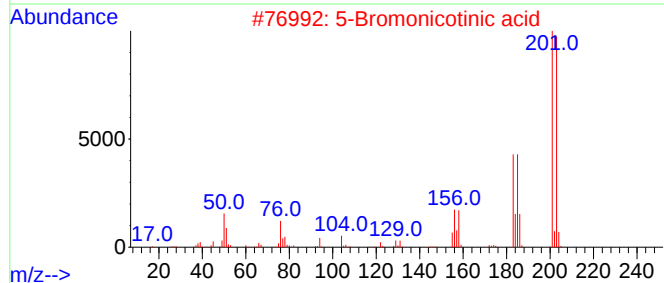
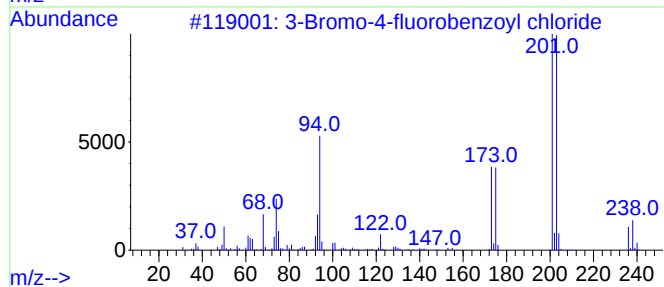
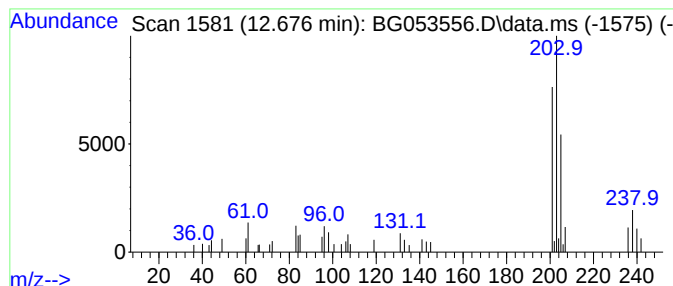
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown12.676 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.676	2.58 ng	45988	Naphthalene-d8	10.896

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Bromo-4-fluorobenzoyl chloride	236	C7H3BrClFO	000672-75-3	43
2		5-Bromonicotinic acid	201	C6H4BrNO2	020826-04-4	43
3		p-Toluic acid, .alpha.,.alpha.,....	238	C8H5Cl3O2	005264-40-4	38
4		4-Amino-5,7-dichlorobenzofurazan	203	C6H3Cl2N3O	330982-41-7	38
5		5-Bromo-2,6-dimethyl-4-pyrimidin...	201	C6H8BrN3	007752-80-9	35



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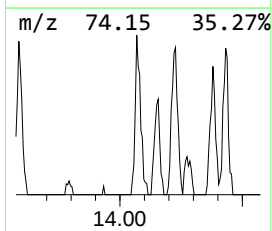
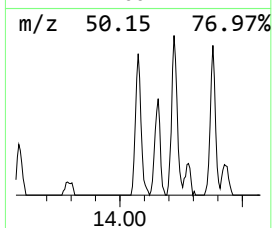
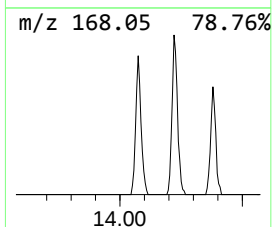
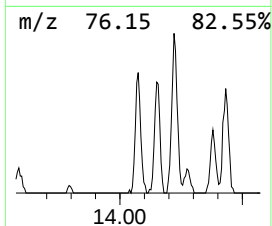
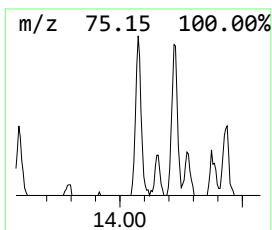
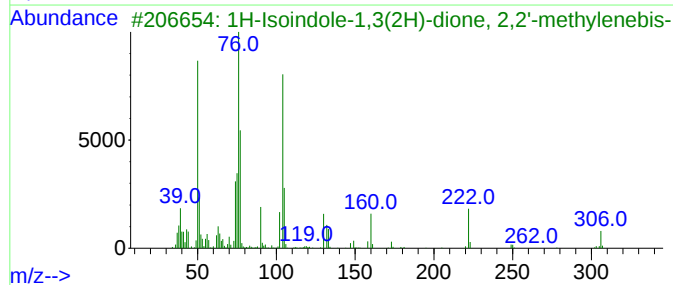
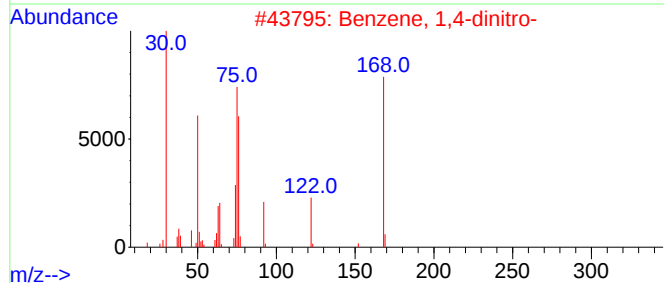
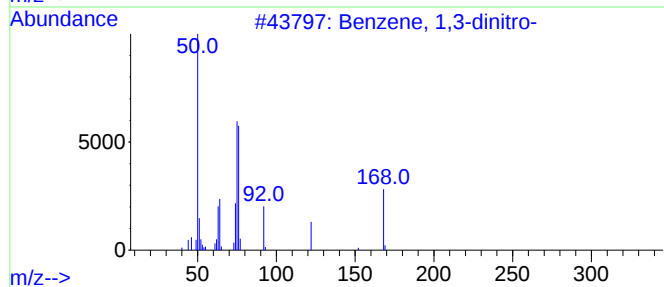
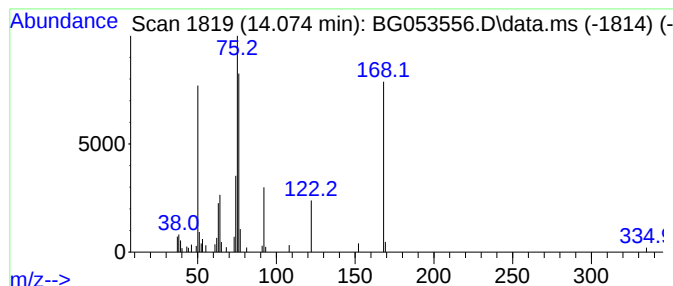
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,3-dinitro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	2.79 ng	67309	Acenaphthene-d10	14.708

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dinitro-	168	C6H4N2O4	000099-65-0	97
2			Benzene, 1,4-dinitro-	168	C6H4N2O4	000100-25-4	95
3			1H-Isoindole-1,3(2H)-dione, 2,2'...	306	C17H10N2O4	033257-56-6	38
4			Phthalimidomethyl 3-methoxybenzoate	311	C17H13NO5	1000224-82-4	37
5			Bicyclo[4.2.0]octa-1,3,5-triene...	132	C8H4O2	006383-11-5	36



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ClientSampleId :
OK-02-051222

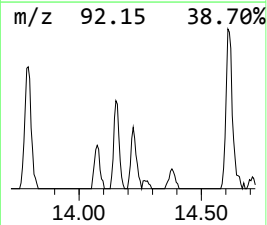
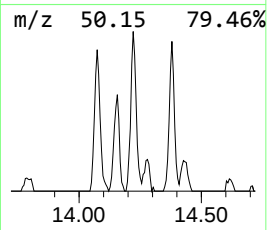
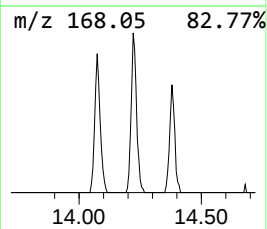
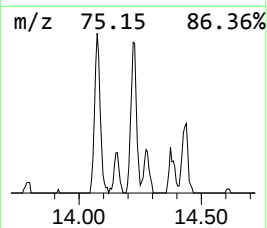
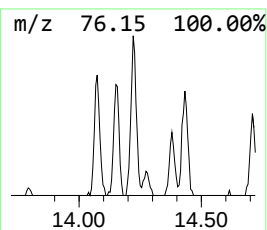
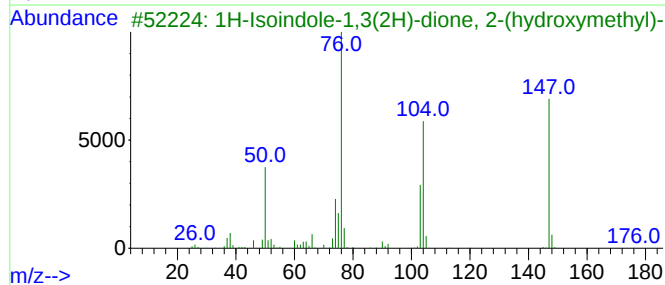
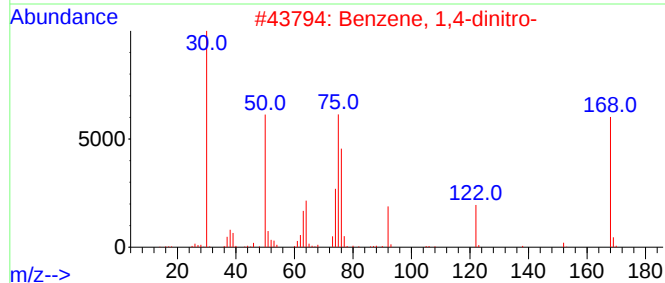
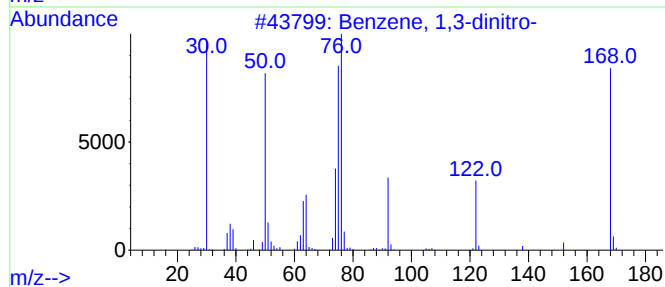
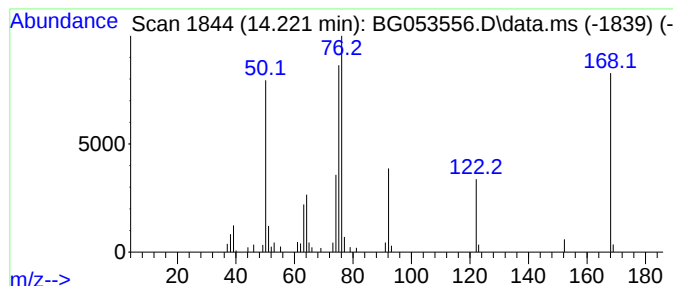
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzene, 1,4-dinitro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	3.17 ng	76509	Acenaphthene-d10	14.708

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dinitro-	168	C6H4N2O4	000099-65-0	95
2			Benzene, 1,4-dinitro-	168	C6H4N2O4	000100-25-4	64
3			1H-Isoindole-1,3(2H)-dione, 2-(h...	177	C9H7N03	000118-29-6	12
4			Benzene, 1,2-dinitro-	168	C6H4N2O4	000528-29-0	9
5			Methyl hydrogen phthalate	180	C9H8O4	004376-18-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053556.D
Acq On : 13 May 2022 23:39
Operator : CG/JU
Sample : N2829-01 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-02-051222

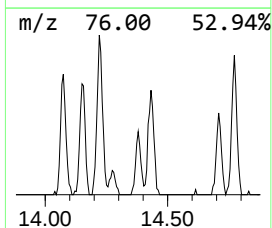
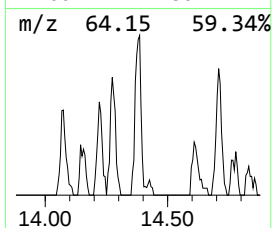
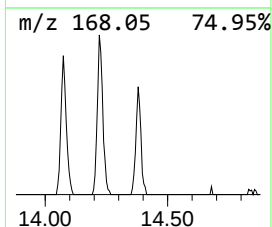
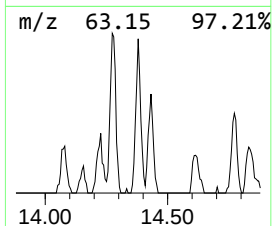
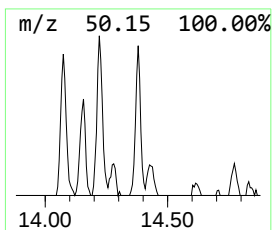
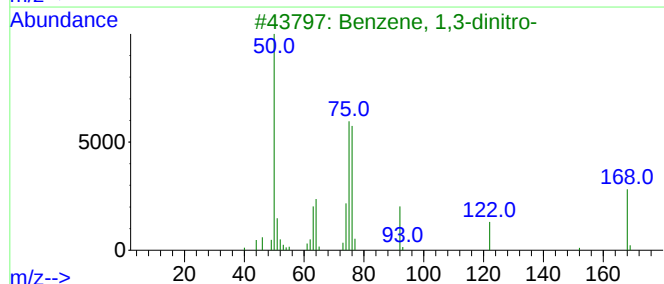
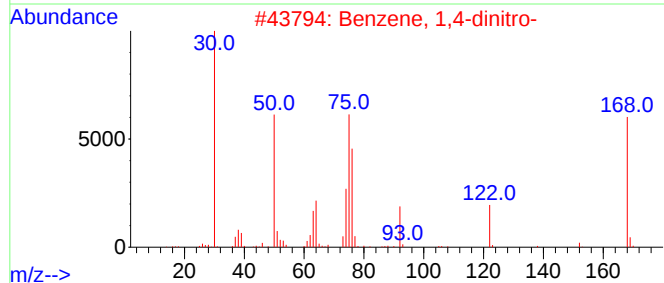
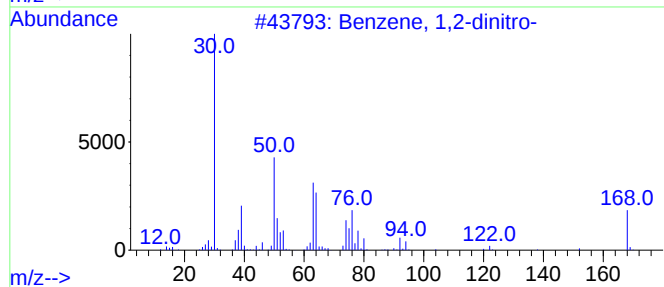
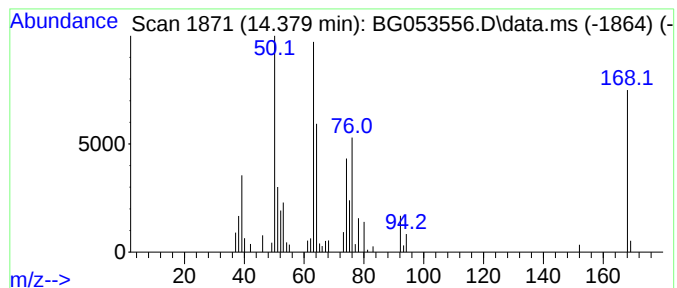
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, 1,2-dinitro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.380	2.71 ng	65383	Acenaphthene-d10	14.708

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-dinitro-	168	C6H4N2O4	000528-29-0	50
2			Benzene, 1,4-dinitro-	168	C6H4N2O4	000100-25-4	45
3			Benzene, 1,3-dinitro-	168	C6H4N2O4	000099-65-0	38
4			Propane, 1,2-dichloro-	112	C3H6Cl2	000078-87-5	10
5			Bicyclo[4.2.0]octa-1,3,5-triene...	132	C8H4O2	006383-11-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053556.D
Acq On : 13 May 2022 23:39
Operator : CG/JU
Sample : N2829-01 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-02-051222

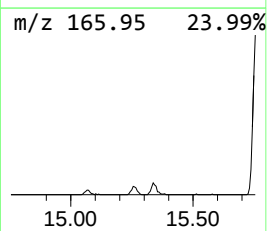
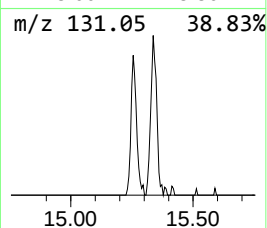
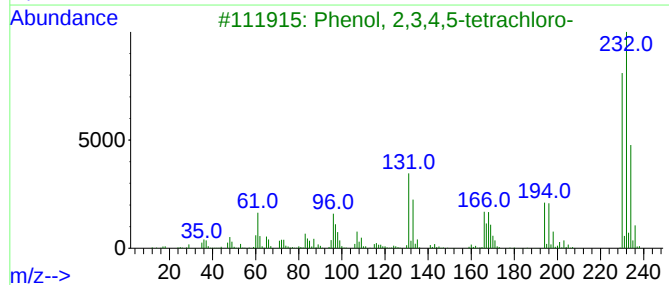
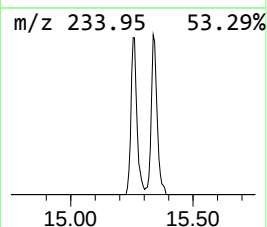
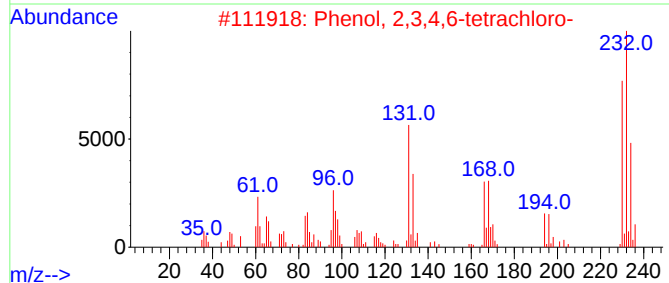
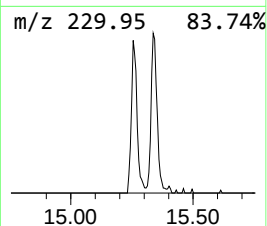
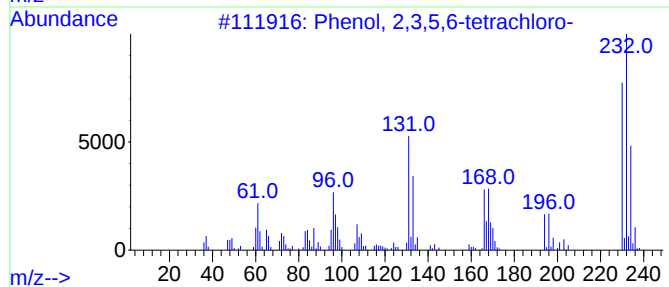
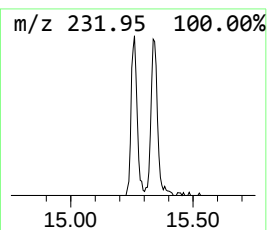
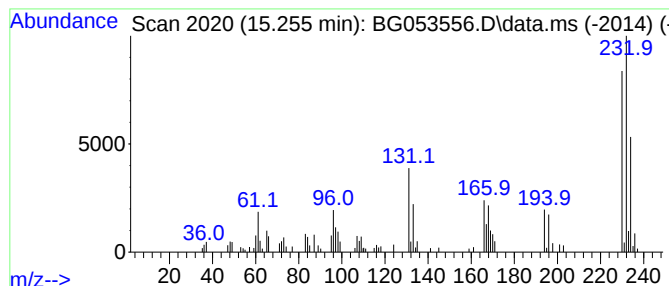
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenol, 2,3,5,6-tetrachloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.255	4.54 ng	109405	Acenaphthene-d10	14.708

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,3,5,6-tetrachloro-	230	C6H2Cl4O	000935-95-5	99
2			Phenol, 2,3,4,6-tetrachloro-	230	C6H2Cl4O	000058-90-2	98
3			Phenol, 2,3,4,5-tetrachloro-	230	C6H2Cl4O	004901-51-3	96
4			4-Aminotetrachloropyridine	230	C5H2Cl4N2	002176-63-8	53
5			2,4,5,6-Tetrachloro-pyridin-3-yl...	230	C5H2Cl4N2	1000277-70-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053556.D
Acq On : 13 May 2022 23:39
Operator : CG/JU
Sample : N2829-01 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-02-051222

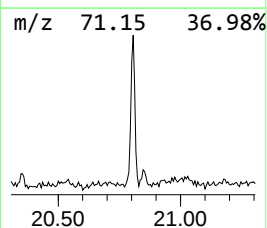
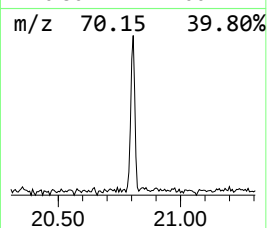
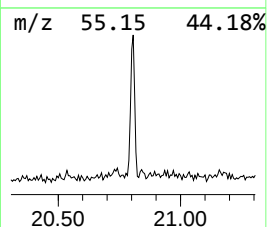
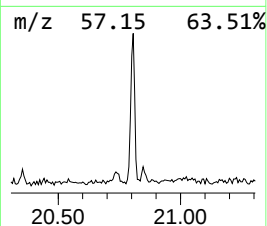
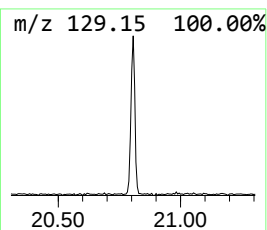
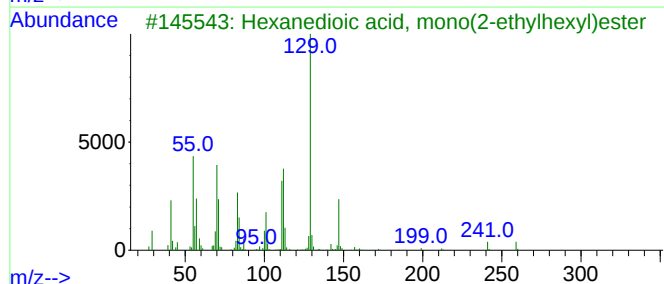
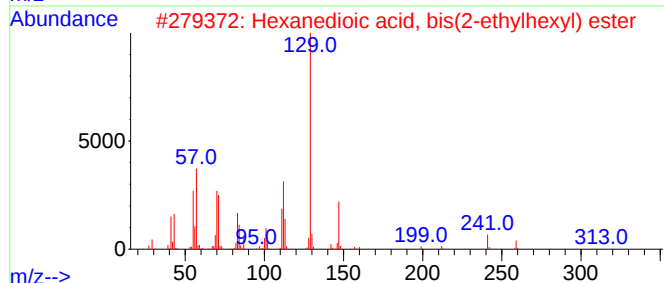
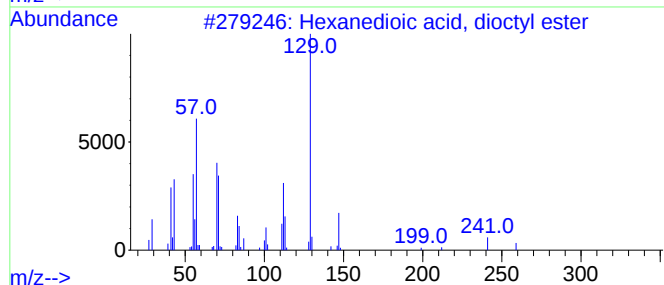
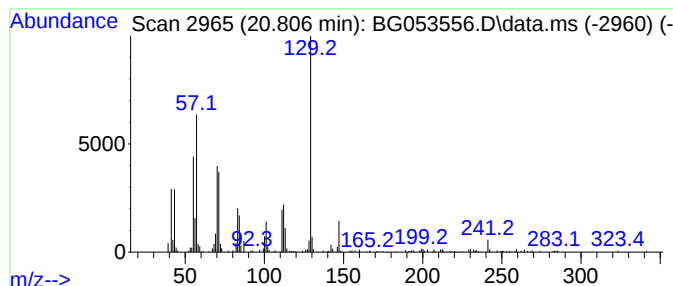
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexanedioic acid, dioctyl e... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.806	4.70 ng	209054	Chrysene-d12	21.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	90
2			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	86
3			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	53
4			Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	50
5			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053556.D
Acq On : 13 May 2022 23:39
Operator : CG/JU
Sample : N2829-01 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-02-051222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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
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unknown12.676	12.676	2.6	ng	45988	2	10.896	355909	20.0
Benzene, 1,3-di...	14.074	2.8	ng	67309	3	14.708	482237	20.0
Benzene, 1,4-di...	14.221	3.2	ng	76509	3	14.708	482237	20.0
Benzene, 1,2-di...	14.380	2.7	ng	65383	3	14.708	482237	20.0
Phenol, 2,3,5,6...	15.255	4.5	ng	109405	3	14.708	482237	20.0
Hexanedioic aci...	20.806	4.7	ng	209054	5	21.734	890502	20.0