

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
 Data File : BG055423.D
 Acq On : 2 Nov 2022 20:32
 Operator : CG/JU
 Sample : N5204-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20071

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-BG110122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055423.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.317	3	5	18	rVB	48515	76893	2.28%	0.149%
2	5.280	333	339	347	rBV	72985	113553	3.37%	0.221%
3	5.767	415	422	430	rBV	388980	632733	18.75%	1.229%
4	7.101	640	649	657	rVB4	15482	40267	1.19%	0.078%
5	7.389	691	698	715	rBV	378718	671179	19.89%	1.303%
6	7.559	718	727	738	rVV2	27084	61794	1.83%	0.120%
7	7.812	763	770	778	rBV	83470	138563	4.11%	0.269%
8	8.241	837	843	849	rBV	119835	195509	5.79%	0.380%
9	8.429	870	875	886	rVB3	22824	56458	1.67%	0.110%
10	8.875	946	951	964	rBV4	14953	42565	1.26%	0.083%
11	9.416	1036	1043	1052	rBV	247673	436318	12.93%	0.847%
12	9.651	1075	1083	1088	rBV	36195	65130	1.93%	0.126%
13	9.710	1088	1093	1104	rVB2	35006	77747	2.30%	0.151%
14	10.021	1140	1146	1155	rVB2	21900	49255	1.46%	0.096%
15	10.403	1205	1211	1215	rBV	24811	40447	1.20%	0.079%
16	10.685	1253	1259	1265	rBV2	23146	45651	1.35%	0.089%
17	11.067	1311	1324	1333	rBV	165775	335492	9.94%	0.652%
18	11.143	1333	1337	1349	rVB3	23832	48717	1.44%	0.095%
19	12.177	1509	1513	1521	rBV3	40609	73423	2.18%	0.143%
20	12.266	1522	1528	1533	rVV	87767	126897	3.76%	0.246%
21	12.618	1584	1588	1591	rBV2	44106	75250	2.23%	0.146%
22	13.000	1646	1653	1657	rBV3	44785	98436	2.92%	0.191%
23	13.165	1676	1681	1688	rBV4	96722	272985	8.09%	0.530%
24	13.270	1695	1699	1708	rVB	173023	314595	9.32%	0.611%
25	13.364	1711	1715	1716	rBV2	97438	122757	3.64%	0.238%
26	13.423	1722	1725	1730	rVB2	165607	227834	6.75%	0.442%
27	13.482	1730	1735	1744	rBV	688918	1149313	34.07%	2.232%
28	13.582	1748	1752	1756	rVV2	107738	167391	4.96%	0.325%
29	13.740	1777	1779	1783	rVB3	57054	60491	1.79%	0.117%
30	13.793	1784	1788	1792	rBV	149344	223738	6.63%	0.434%
31	13.893	1798	1805	1811	rVB2	598805	1352936	40.10%	2.627%
32	13.952	1812	1815	1817	rBV	74684	96608	2.86%	0.188%
33	13.987	1817	1821	1826	rVV2	177217	309892	9.19%	0.602%
34	14.040	1827	1830	1834	rVB2	119409	153705	4.56%	0.298%
35	14.093	1836	1839	1842	rVB	72337	83198	2.47%	0.162%
36	14.134	1843	1846	1849	rBV2	78216	100569	2.98%	0.195%

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37	14.210	1856	1859	1870	rVB3	96715	164165	4.87%	0.319%
38	14.304	1871	1875	1879	rVB	150467	185560	5.50%	0.360%
39	14.563	1917	1919	1922	rBV	50248	47678	1.41%	0.093%
40	14.780	1952	1956	1961	rBV	567395	836337	24.79%	1.624%
41	14.863	1965	1970	1974	rBV2	437911	695845	20.62%	1.351%
42	14.998	1990	1993	1997	rVB2	232240	287328	8.52%	0.558%
43	15.215	2028	2030	2034	rBV2	108230	112379	3.33%	0.218%
44	15.650	2100	2104	2109	rVB	258310	552792	16.38%	1.074%
45	15.761	2119	2123	2128	rVB	879933	1123050	33.29%	2.181%
46	15.861	2138	2140	2144	rVB2	271021	300090	8.89%	0.583%
47	16.502	2247	2249	2254	rVB2	829909	956426	28.35%	1.857%
48	16.966	2323	2328	2334	rVB	2330083	3373822	100.00%	6.552%
49	17.031	2335	2339	2343	rVB	907884	1179360	34.96%	2.290%
50	17.642	2439	2443	2448	rVB	1630807	2262223	67.05%	4.393%
51	17.712	2451	2455	2461	rVB2	725508	1153033	34.18%	2.239%
52	18.358	2560	2565	2572	rVB2	1560148	2568275	76.12%	4.988%
53	18.922	2658	2661	2665	rBV	1311933	1810162	53.65%	3.515%
54	18.964	2666	2668	2672	rVB	1194410	1263352	37.45%	2.453%
55	19.298	2721	2725	2732	rVV	2198589	3060547	90.71%	5.944%
56	19.363	2733	2736	2742	rVB	1046389	1427825	42.32%	2.773%
57	19.833	2812	2816	2820	rBV	1678971	2098931	62.21%	4.076%
58	19.898	2824	2827	2829	rBV	654092	724153	21.46%	1.406%
59	20.168	2870	2873	2879	rVB	928787	1204626	35.71%	2.339%
60	20.356	2902	2905	2909	rVB	1237318	1499287	44.44%	2.912%
61	20.838	2984	2987	2993	rVB	971558	1266095	37.53%	2.459%
62	21.102	3028	3032	3036	rVB	1960398	2415112	71.58%	4.690%
63	21.173	3041	3044	3052	rVB	981344	1387953	41.14%	2.695%
64	21.619	3115	3120	3127	rVV	1409877	2139655	63.42%	4.155%
65	21.696	3129	3133	3141	rVB2	782557	1455984	43.16%	2.827%
66	22.172	3211	3214	3222	rVB	953081	1515359	44.92%	2.943%
67	23.165	3378	3383	3392	rVB	1458336	2649259	78.52%	5.145%
68	23.946	3511	3516	3523	rVB	798513	1638780	48.57%	3.182%

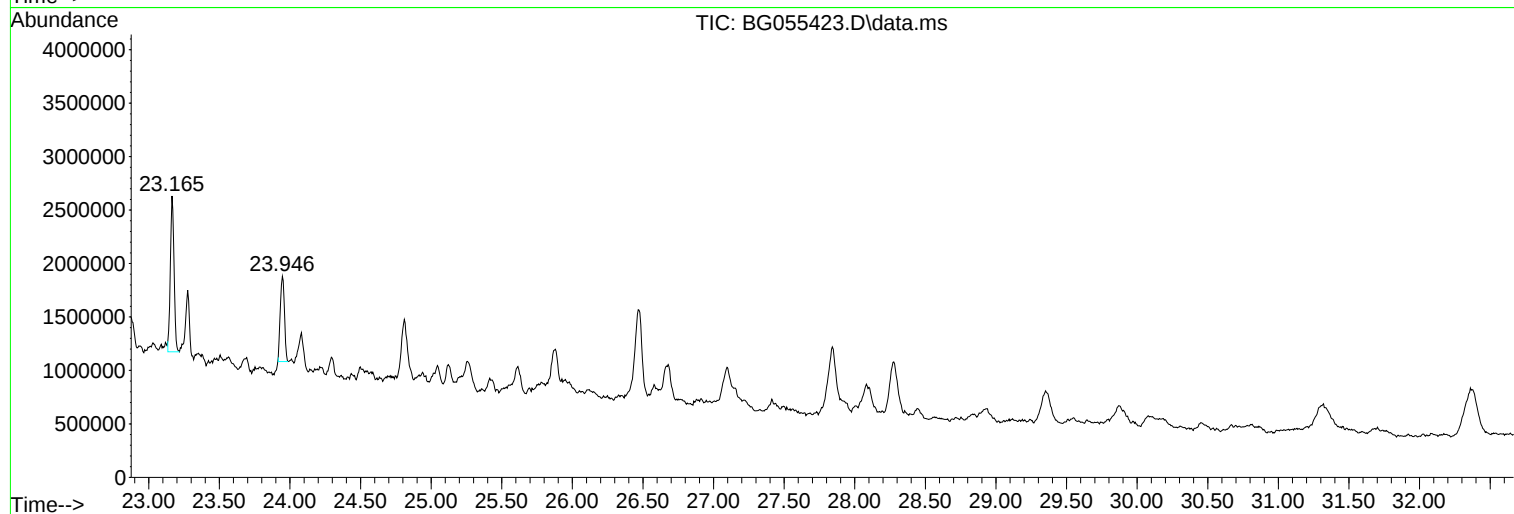
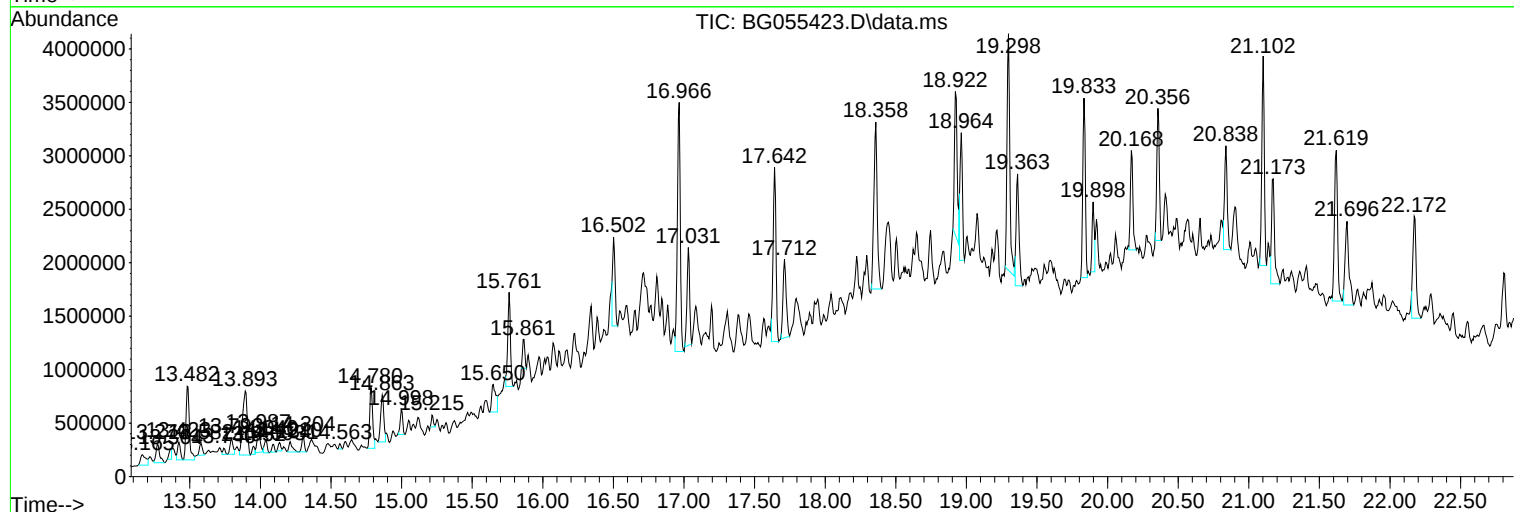
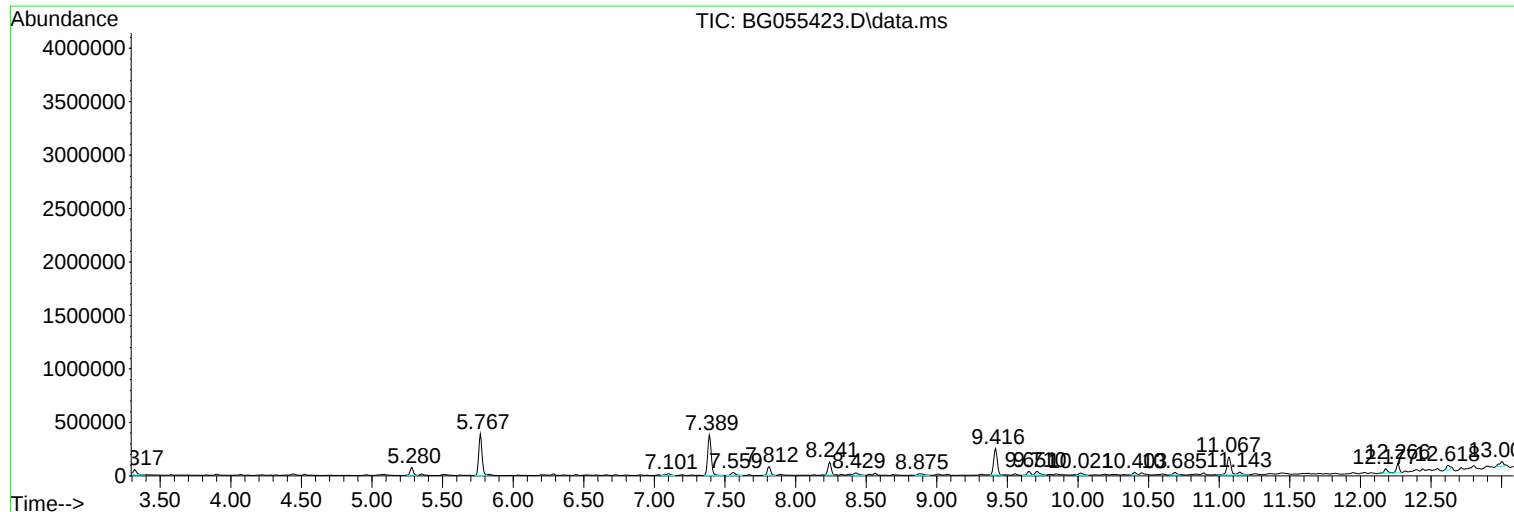
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
BNA_G
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20071

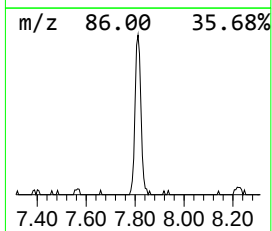
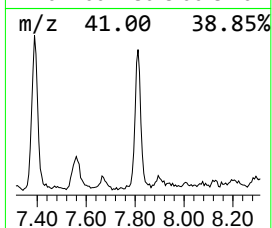
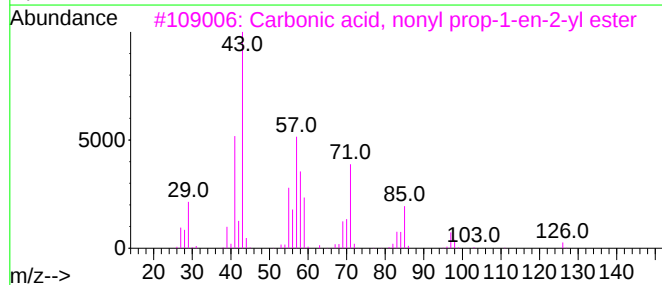
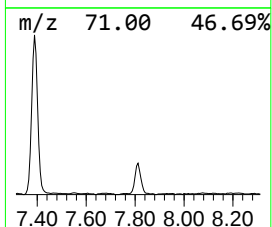
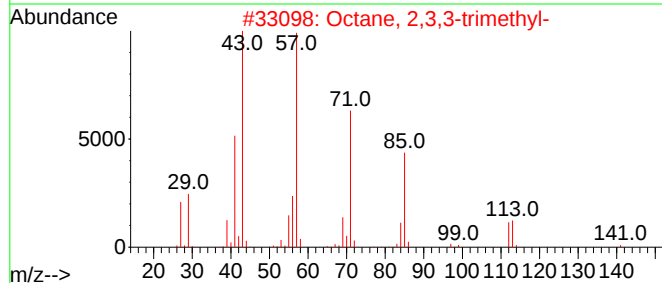
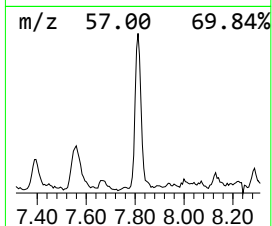
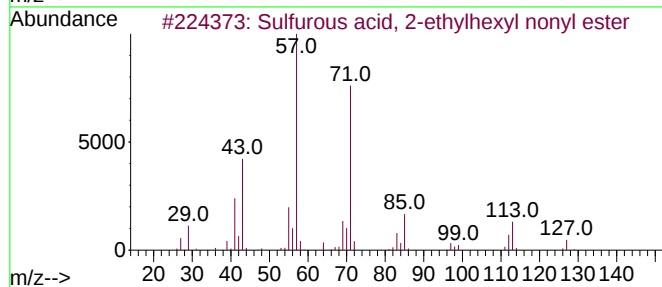
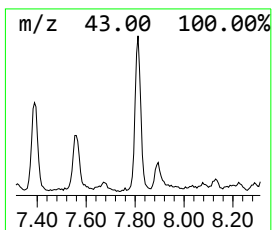
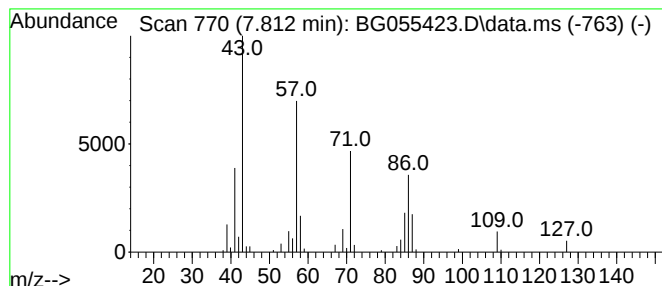
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.812 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.812	14.17 ng	138563	1,4-Dichlorobenzene-d4	8.241

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	38
2			Octane, 2,3,3-trimethyl-	156	C11H24	062016-30-2	38
3			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	37
4			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	37
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	37



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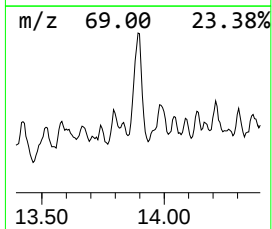
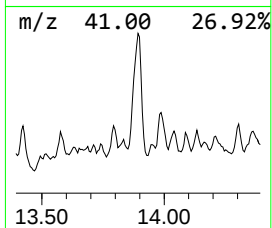
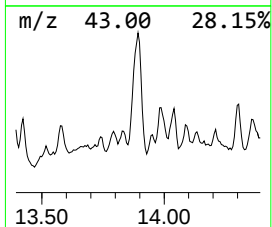
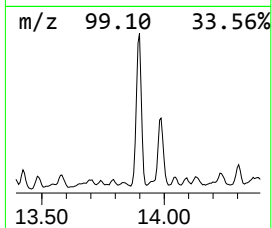
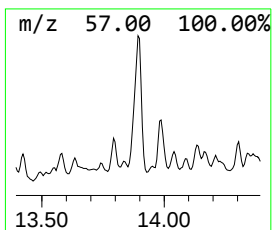
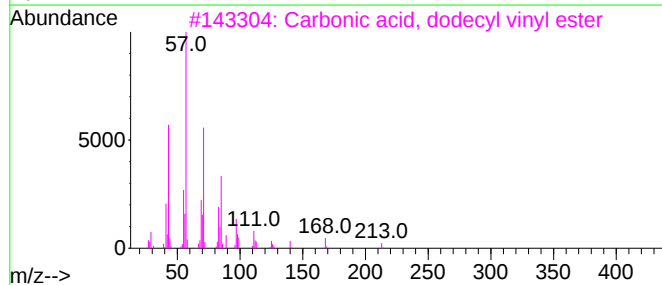
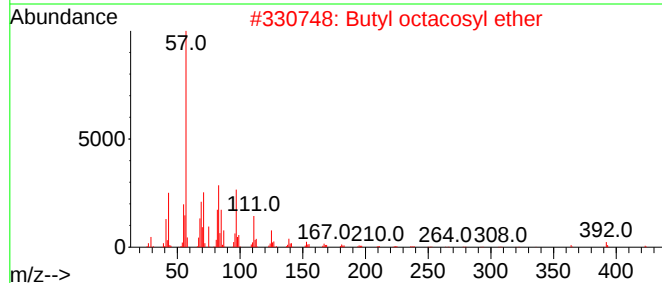
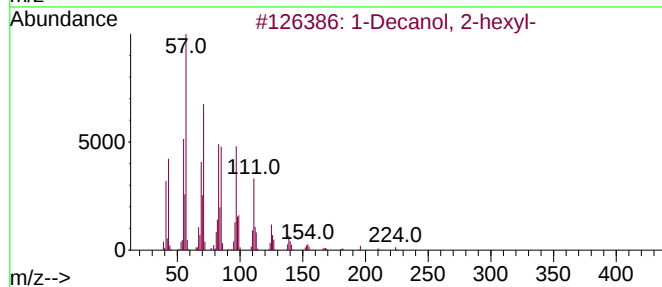
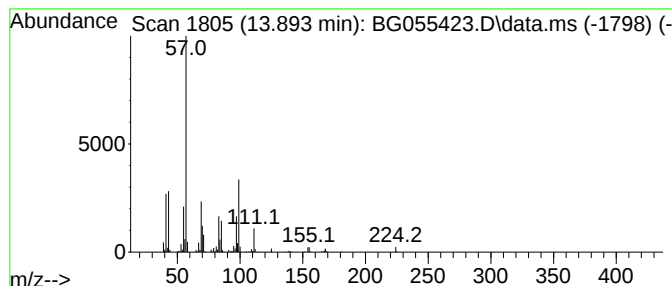
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Decanol, 2-hexyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.893	38.89 ng	1352940	Acenaphthene-d10	14.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-			242	C16H34O	002425-77-6	64
2	Butyl octacosyl ether			467	C32H66O	1000406-41-1	53
3	Carbonic acid, dodecyl vinyl ester			256	C15H28O3	1000382-54-8	50
4	Pentafluoropropionic acid, tetra...			360	C17H29F5O2	006222-06-6	47
5	9-Eicosene, (E)-			280	C20H40	074685-29-3	43



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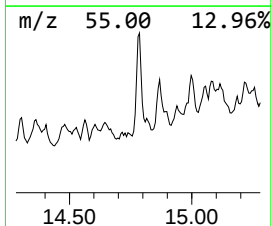
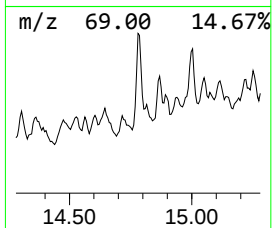
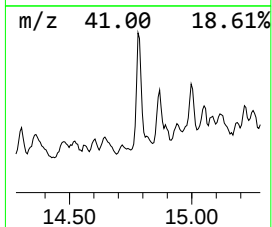
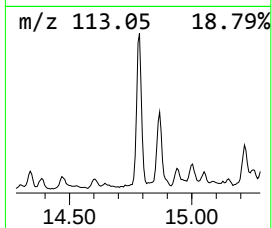
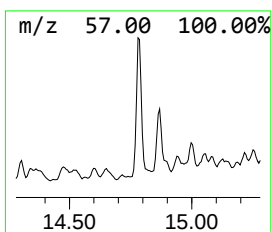
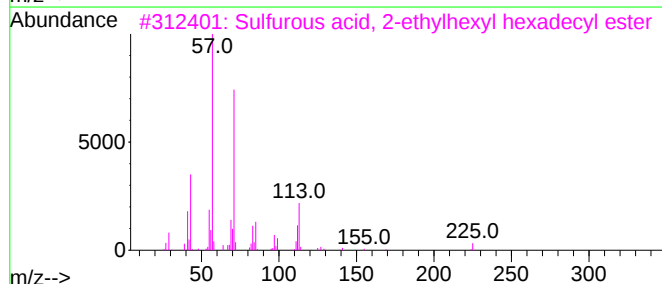
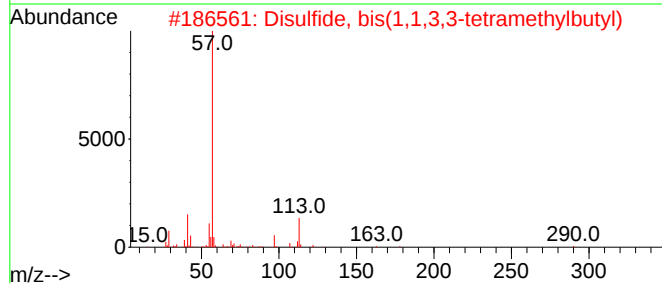
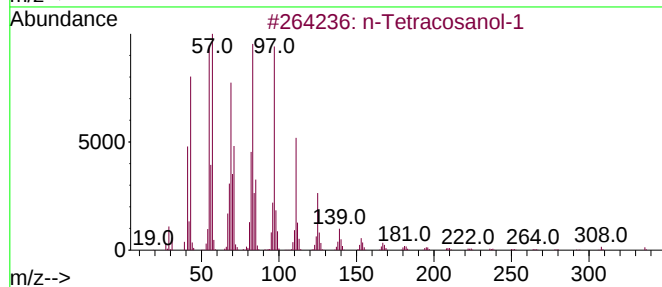
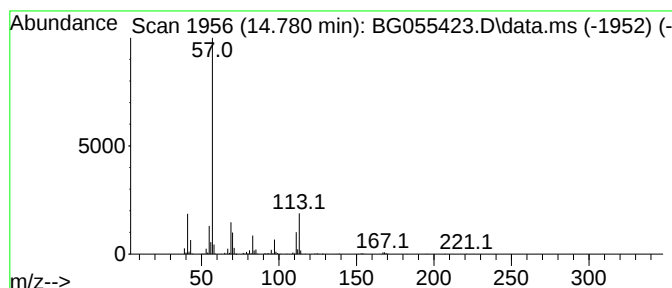
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Peak Number 3 unknown14.780 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	24.04 ng	836337	Acenaphthene-d10	14.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	47
2			Disulfide, bis(1,1,3,3-tetrameth...	290	C16H34S2	029956-99-8	43
3			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	39
4			Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	38
5			Carbonic acid, but-2-yn-1-yl oct...	366	C23H42O3	1000383-21-3	38



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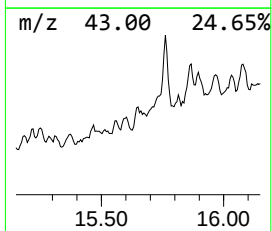
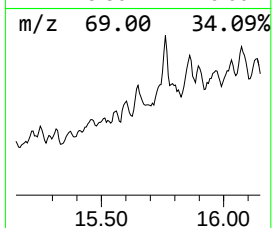
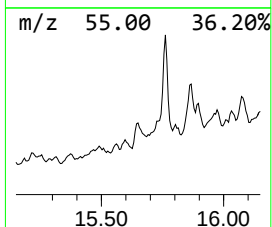
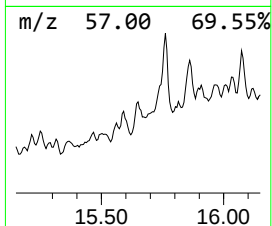
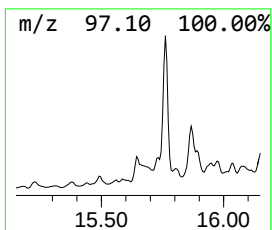
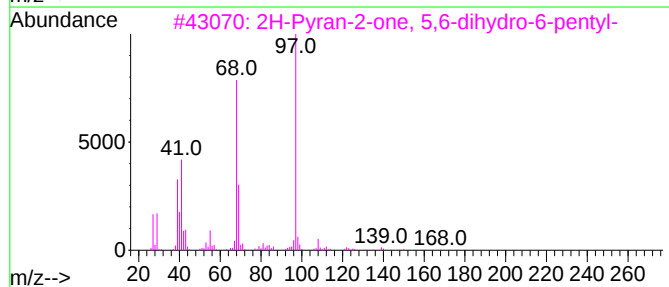
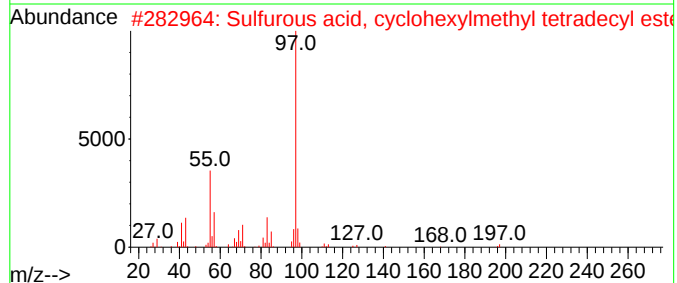
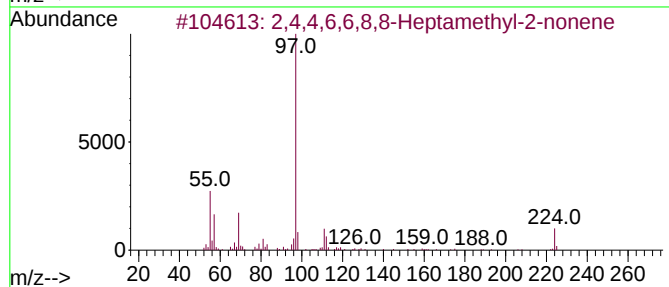
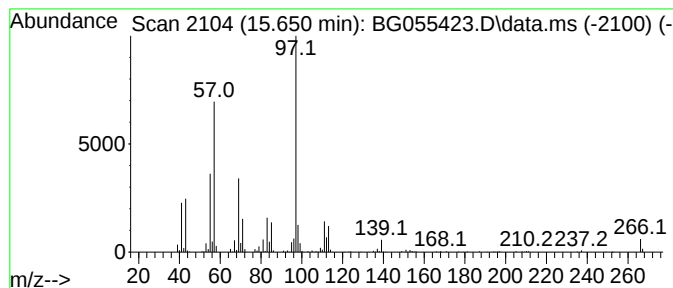
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2,4,4,6,6,8,8-Heptamethyl-2... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.650	15.89 ng	552792	Acenaphthene-d10	14.857	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-2-nonene	224	C16H32	039761-73-4	59
2	Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	59
3	2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	53
4	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	53
5	Sulfurous acid, cyclohexylmethyl...	360	C20H40O3S	1000309-22-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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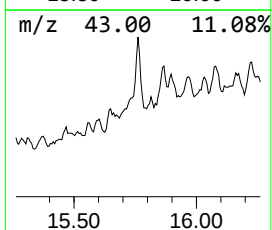
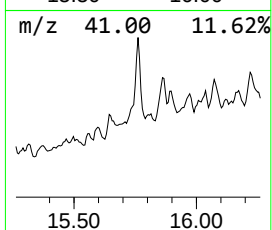
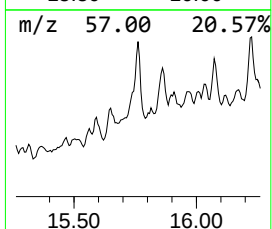
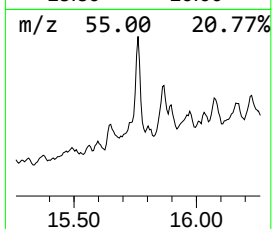
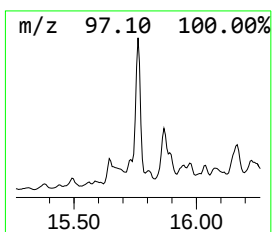
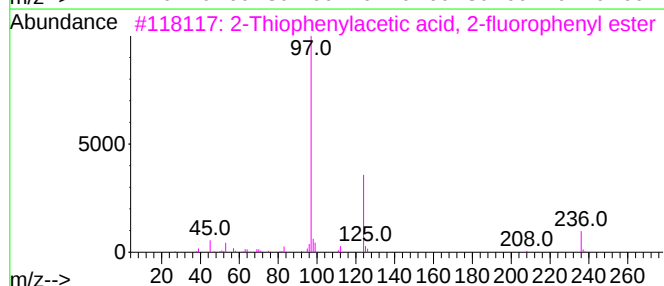
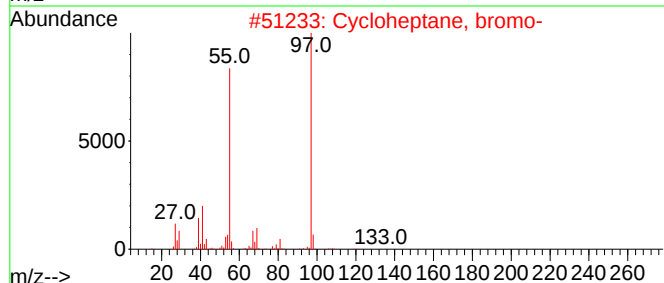
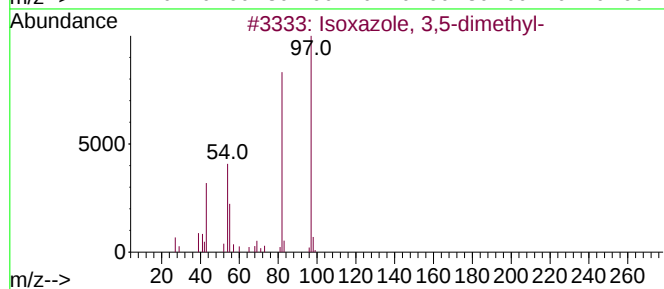
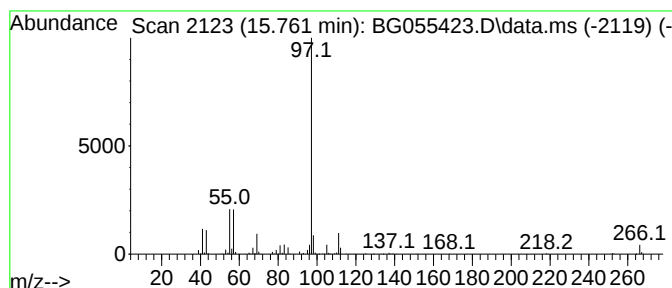
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Isoxazole, 3,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.762	32.28 ng	1123050	Acenaphthene-d10	14.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	59
2			Cycloheptane, bromo-	176	C7H13Br	002404-35-5	45
3			2-Thiophenylacetic acid, 2-fluor...	236	C12H9FO2S	1000325-71-6	45
4			2-Thiopheneacetic acid, 1-cyclop...	238	C13H18O2S	1000278-96-0	39
5			2H-Pyran-4-carboxylic acid, 3,4-...	170	C9H14O3	038858-64-9	39



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
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Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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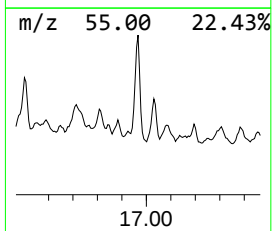
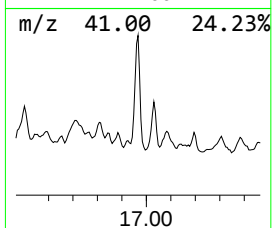
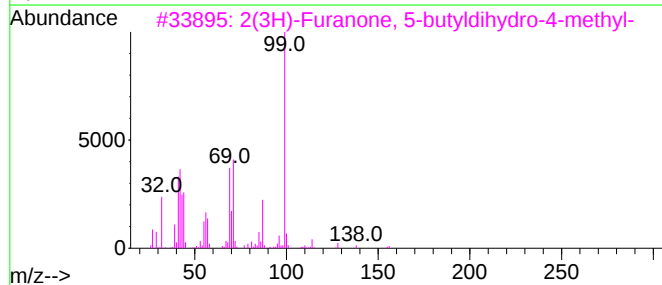
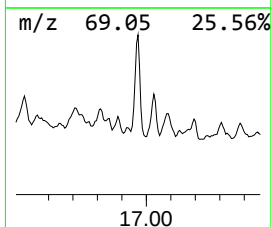
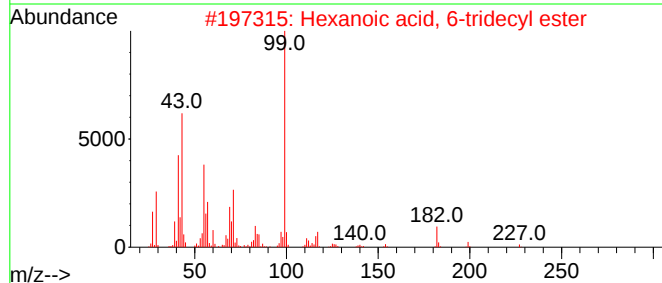
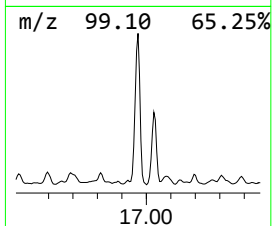
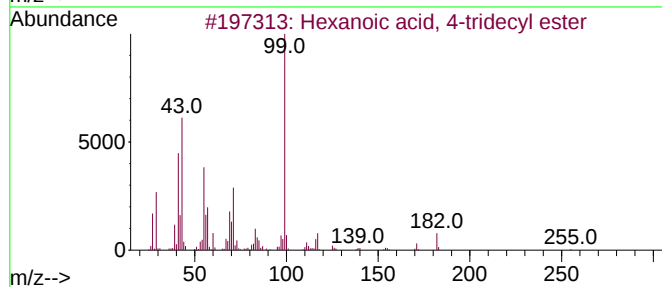
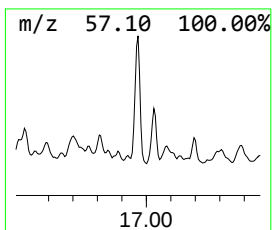
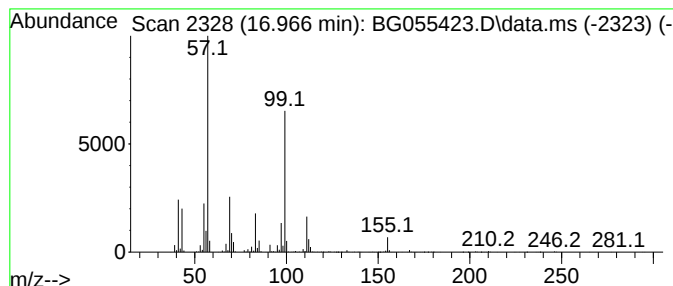
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.966 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.966	29.83 ng	3373820	Phenanthrene-d10	17.595

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	47
2			Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	47
3			2(3H)-Furanone, 5-butyldihydro-4...	156	C9H16O2	039212-23-2	43
4			Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	40
5			Hexanoic acid, 4-tetradecyl ester	312	C20H40O2	1000279-29-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
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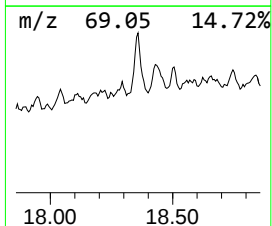
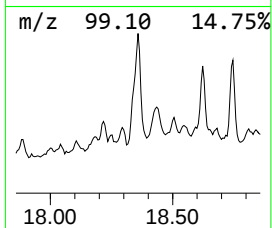
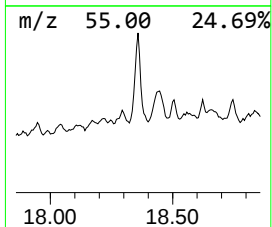
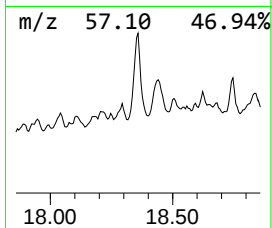
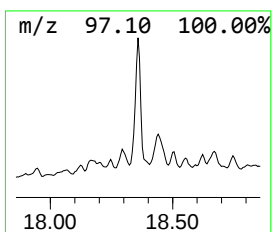
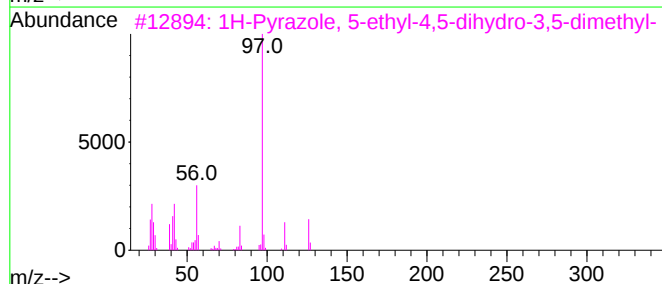
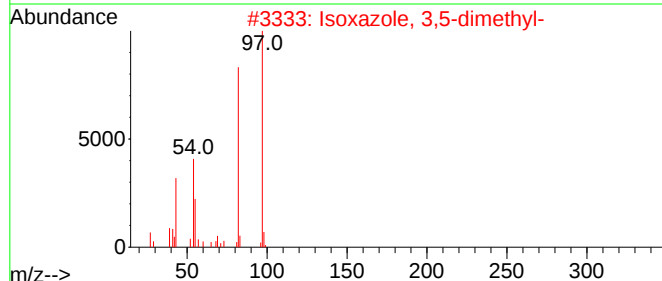
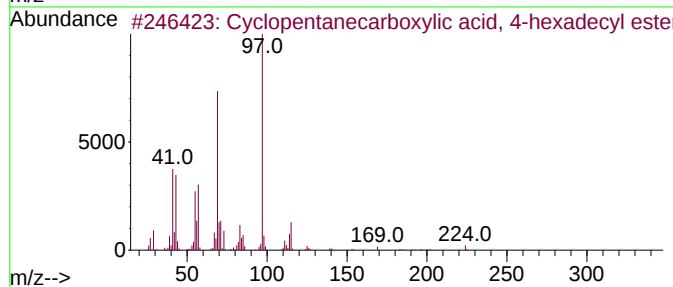
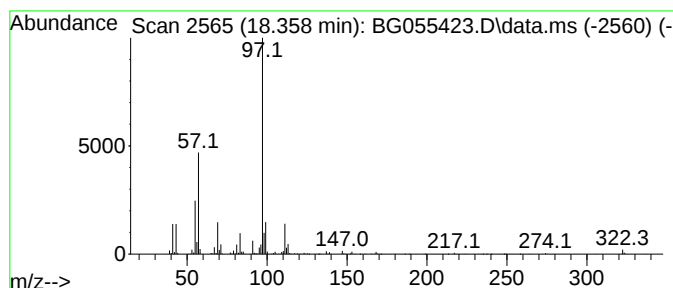
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopentanecarboxylic acid... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.358	22.71 ng	2568280	Phenanthrene-d10		17.595	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxylic acid, 4-h...		338	C22H42O2	1000282-77-5	64
2	Isoxazole, 3,5-dimethyl-		97	C5H7NO	000300-87-8	59
3	1H-Pyrazole, 5-ethyl-4,5-dihydro...		126	C7H14N2	021981-22-6	59
4	Cyclohexene, 1-(1,1-dimethyletho...		168	C11H20O	040648-24-6	53
5	2-Thiopheneacetic acid, 1-cyclop...		238	C13H18O2S	1000278-96-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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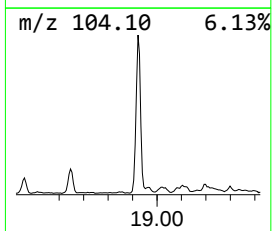
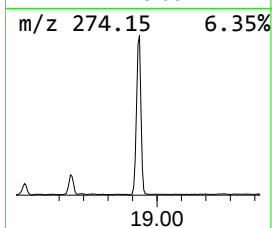
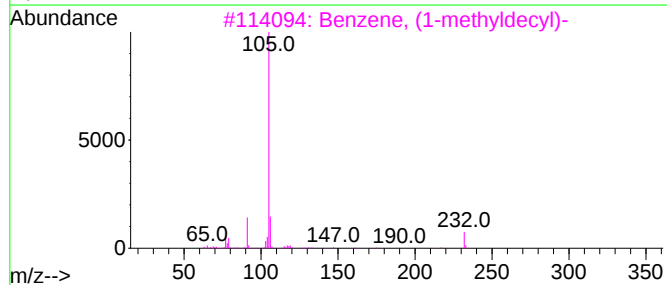
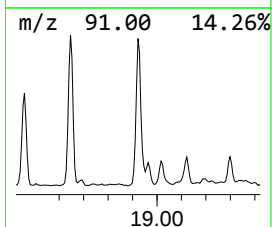
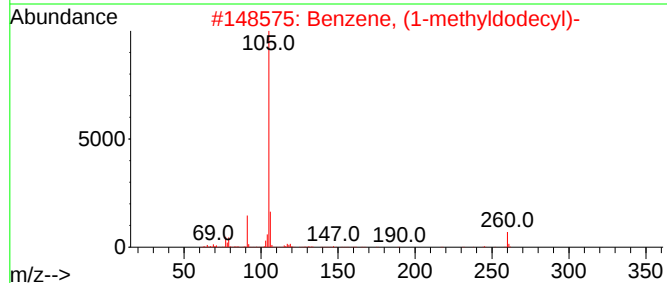
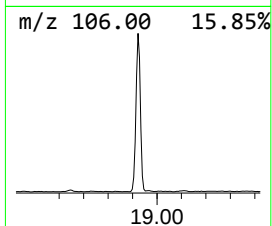
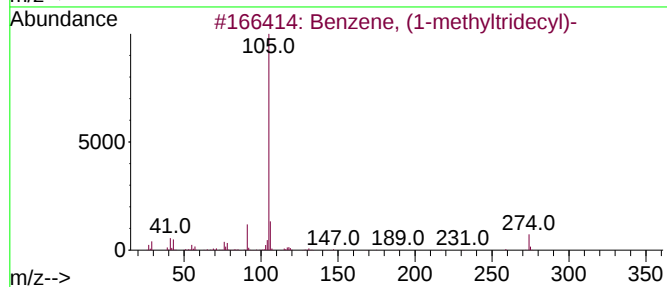
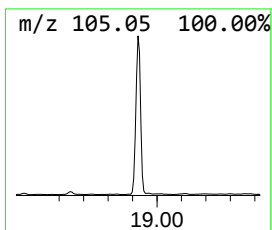
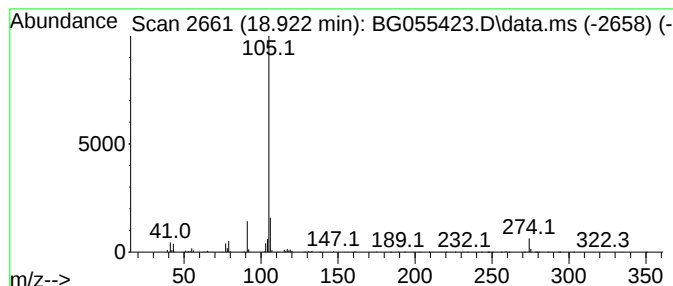
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzene, (1-methyltridecyl)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.922	16.00 ng	1810160	Phenanthrene-d10	17.595

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	91
2			Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	87
3			Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	87
4			Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	72
5			Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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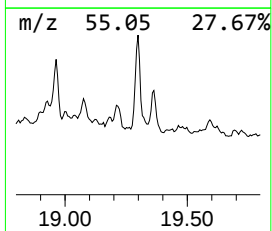
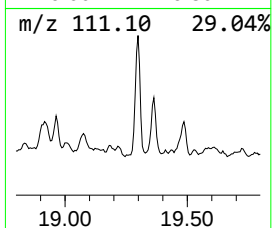
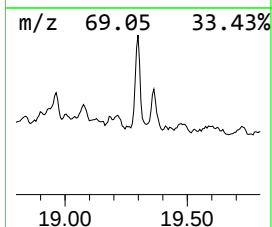
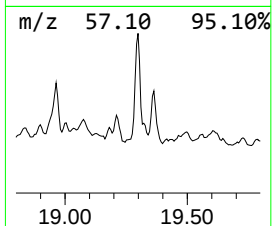
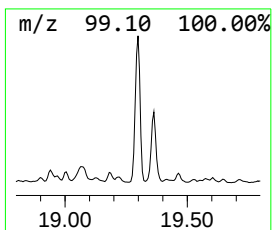
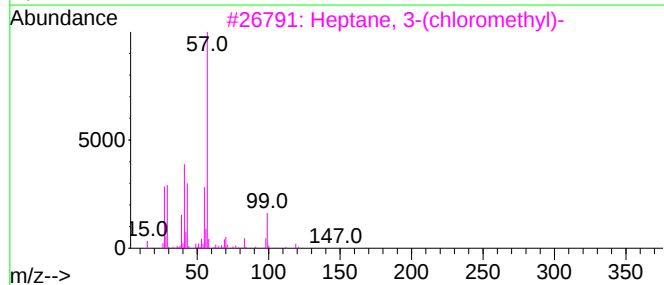
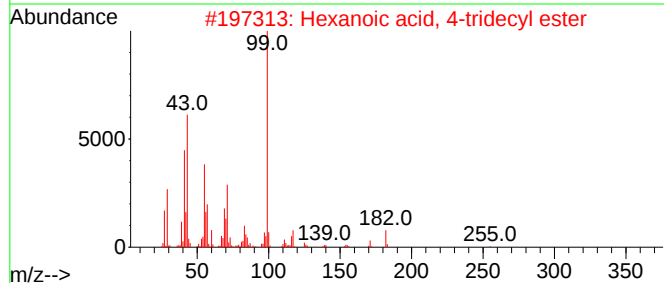
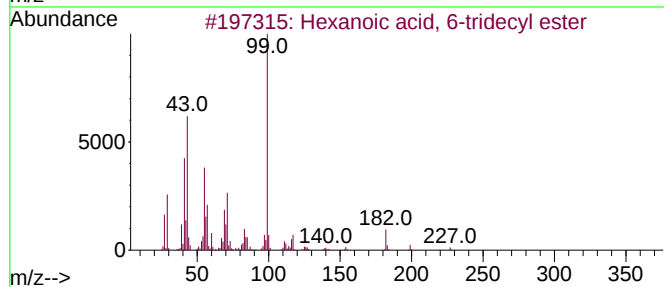
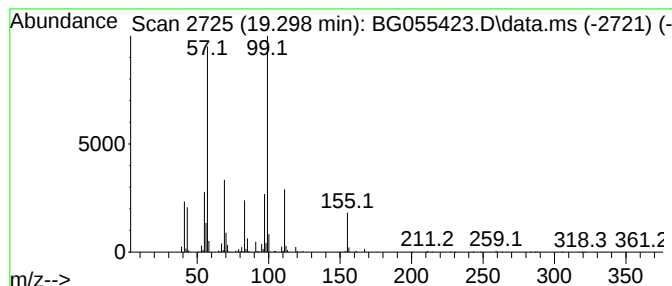
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown19.299 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.299	27.06 ng	3060550	Phenanthrene-d10	17.595

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	43
2			Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	43
3			Heptane, 3-(chloromethyl)-	148	C8H17Cl	000123-04-6	38
4			Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	38
5			Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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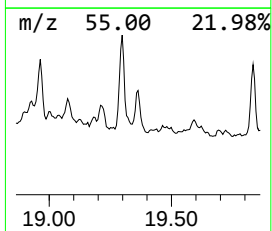
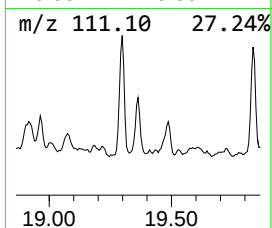
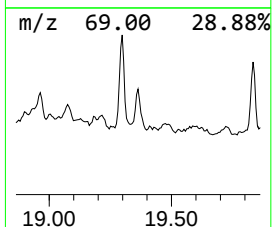
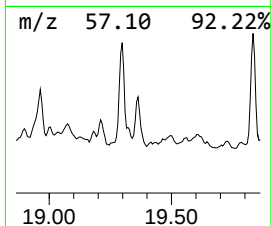
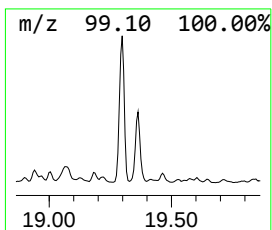
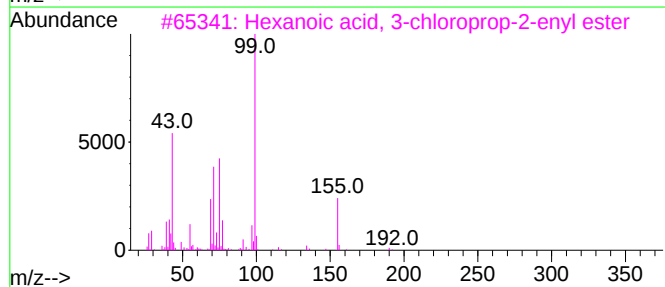
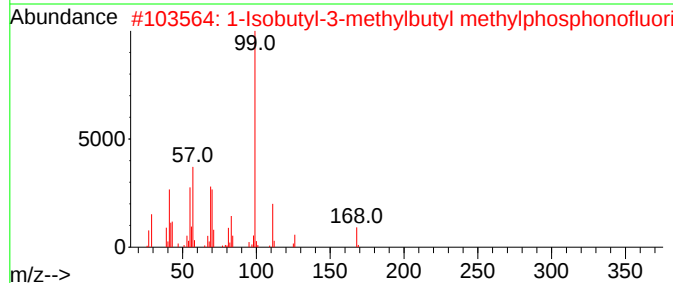
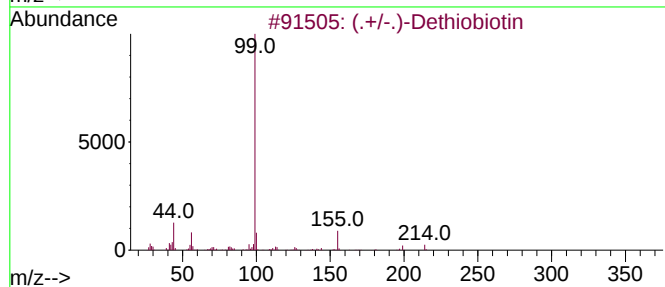
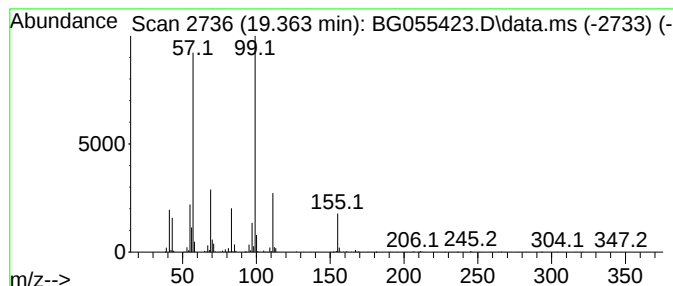
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown19.363 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.363	12.62 ng	1427830	Phenanthrene-d10	17.595

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(./-.)		Dethiobiotin	214	C10H18N2O3	000636-20-4	47
2	1-Isobutyl-3-methylbutyl methylp...			224	C10H22F02P	193090-16-3	42
3	Hexanoic acid, 3-chloroprop-2-en...			190	C9H15ClO2	1000299-36-1	38
4	Fumaric acid, 2,4,4-trimethylpen...			372	C18H22Cl2O4	1000405-61-1	38
5	Fumaric acid, 2,4,4-trimethylpen...			356	C18H22ClF04	1000405-60-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
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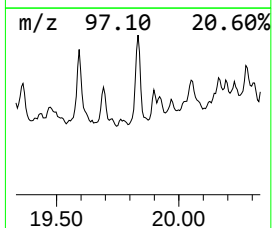
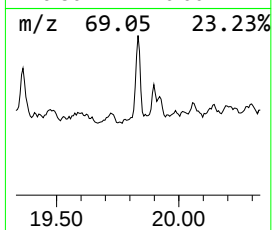
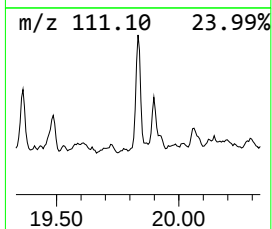
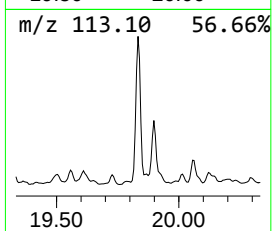
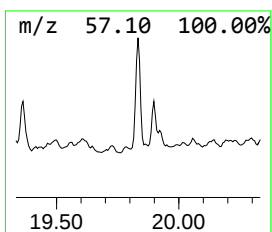
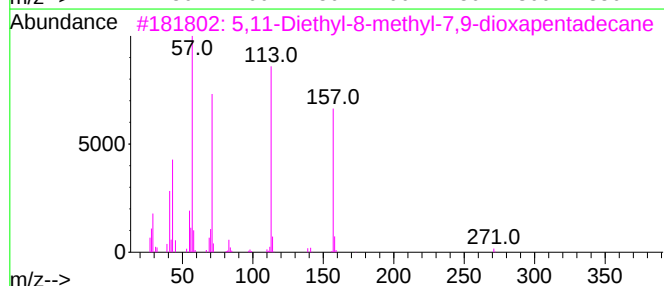
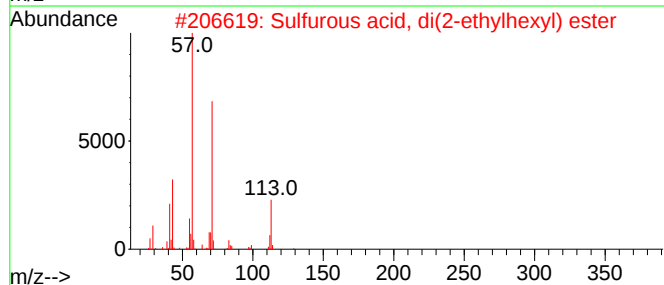
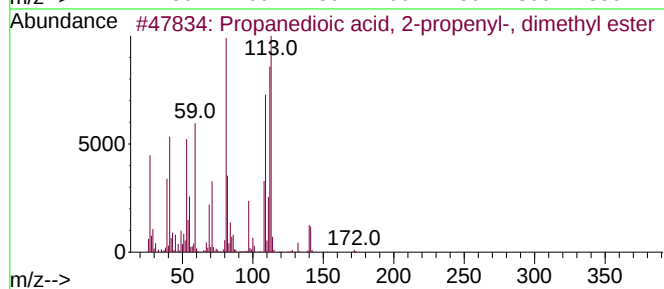
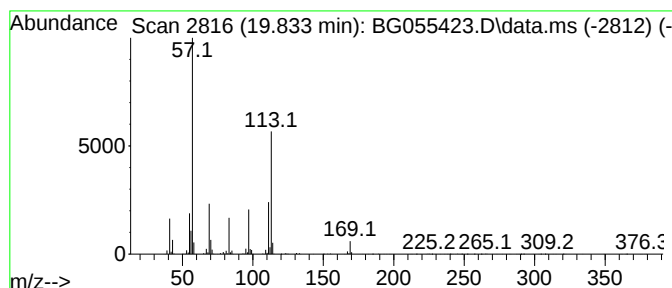
Instrument :
BNA_G
ClientSampleId :
20071

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown19.833 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.833	28.83 ng	2098930	Chrysene-d12	21.872
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		Propanedioic acid, 2-propenyl-, ...	172 C8H12O4	040637-56-7 47
2		Sulfurous acid, di(2-ethylhexyl)...	306 C16H34O3S	1000309-19-1 38
3		5,11-Diethyl-8-methyl-7,9-dioxap...	286 C18H38O2	1000334-83-1 28
4		1-Heptacosanol	396 C27H56O	002004-39-9 25
5		Ethyl 3-[(4-ethylpiperazin-1-yl)...	330 C13H22N4O4S	1000514-46-7 25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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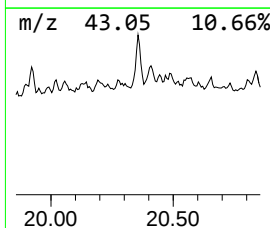
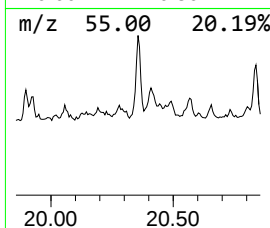
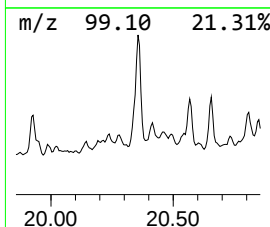
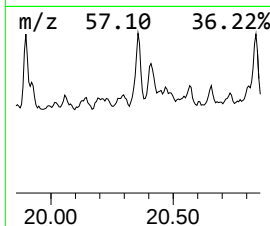
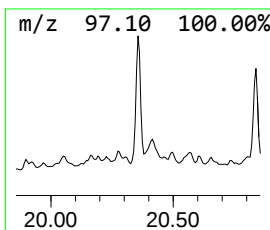
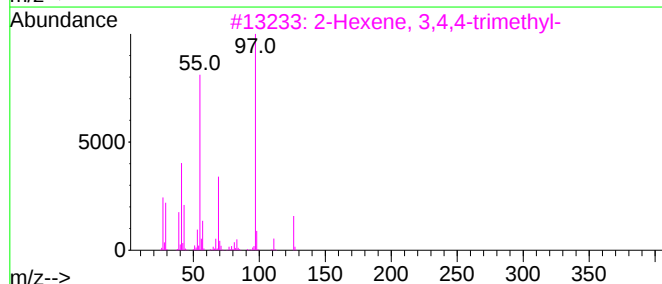
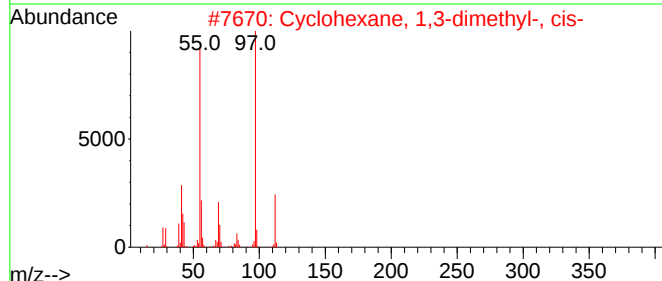
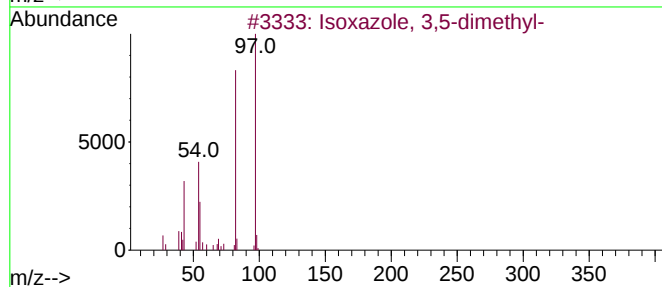
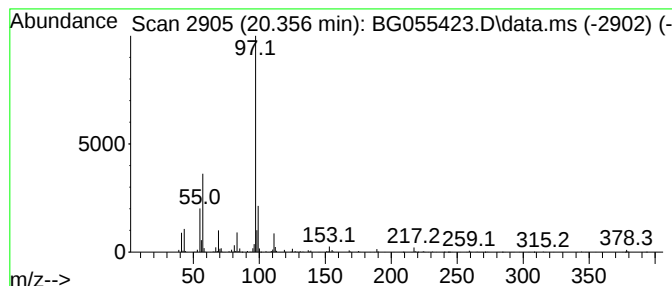
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.356	20.59 ng	1499290	Chrysene-d12	21.872

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	64
2			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	53
3			2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	45
4			Cyclohexanone, 3-butyl-	154	C10H18O	039178-69-3	45
5			Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

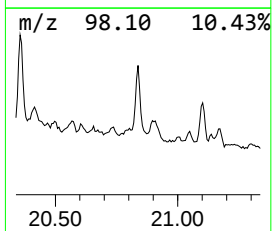
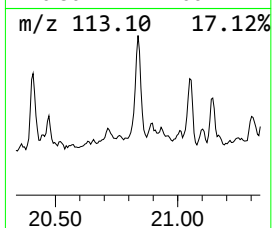
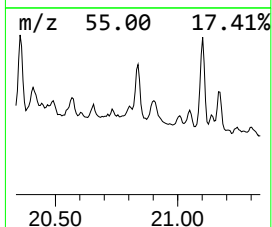
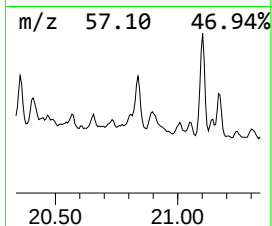
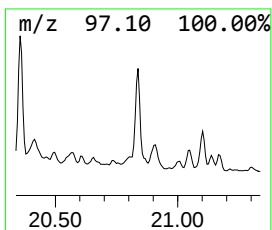
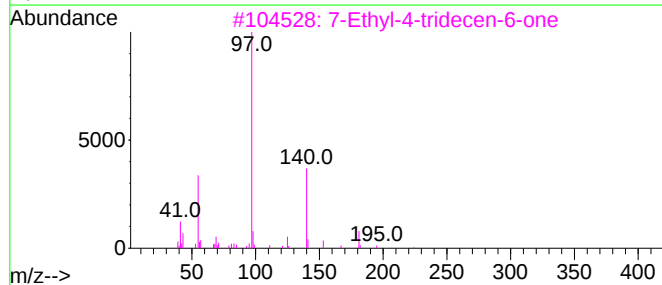
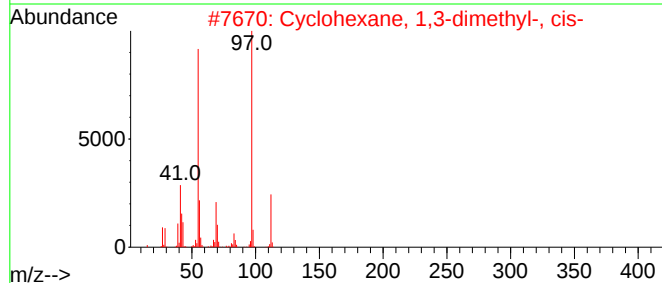
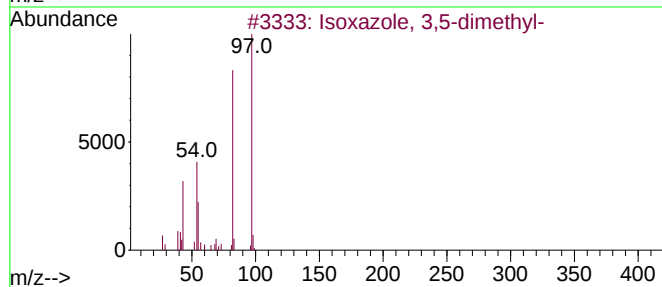
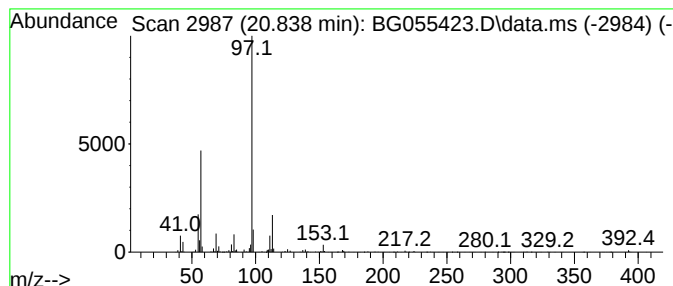
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 7-Ethyl-4-tridecen-6-one Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.838	17.39 ng	1266100	Chrysene-d12		21.872	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Isoxazole, 3,5-dimethyl-		97	C5H7NO	000300-87-8	64
2	Cyclohexane, 1,3-dimethyl-, cis-		112	C8H16	000638-04-0	59
3	7-Ethyl-4-tridecen-6-one		224	C15H28O	1010374-07-1	59
4	4-Methyl-2,3-hexadien-1-ol		112	C7H12O	1000196-09-6	50
5	2-Hexene, 3,4,4-trimethyl-		126	C9H18	053941-19-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20071

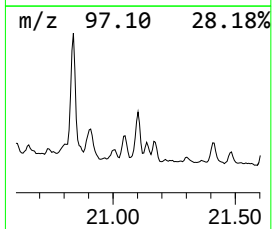
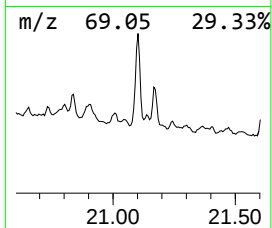
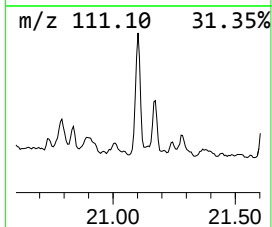
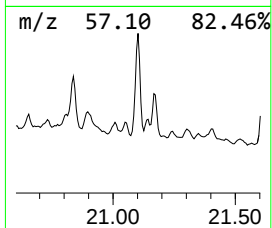
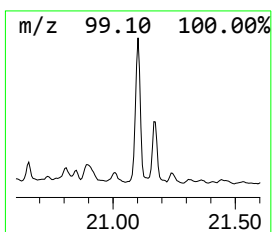
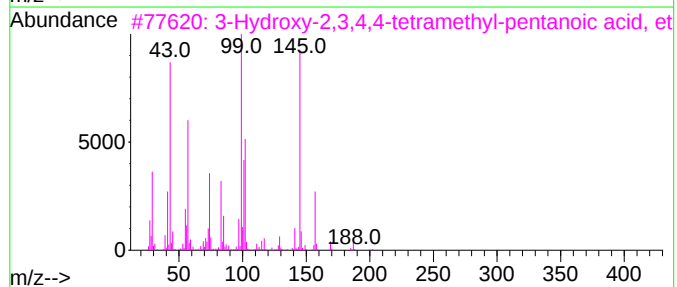
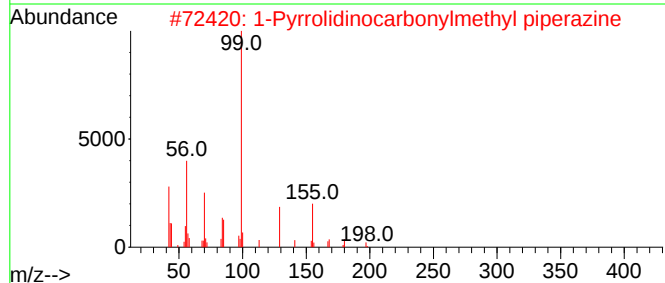
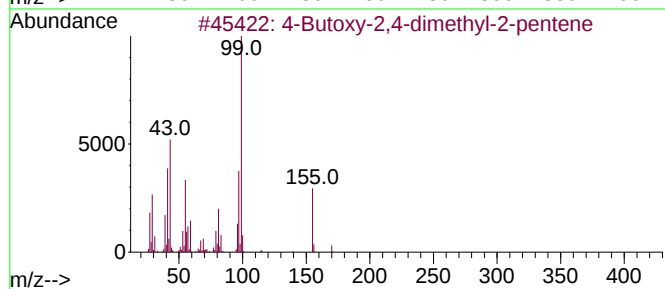
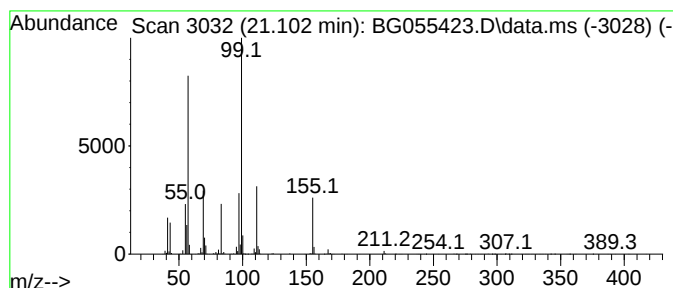
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 4-Butoxy-2,4-dimethyl-2-pen... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.102	33.17 ng	2415110	Chrysene-d12	21.872

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	53
2			1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	38
3			3-Hydroxy-2,3,4,4-tetramethyl-pe...	202	C11H22O3	1000194-64-5	38
4			Tributyl phosphate	266	C12H27O4P	000126-73-8	38
5			2,4,4-Trimethyl-1-pentyl methylp...	210	C9H20FO2P	333416-06-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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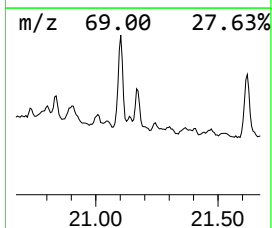
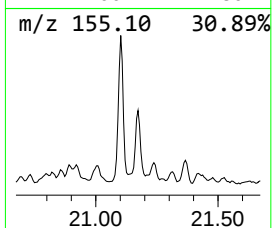
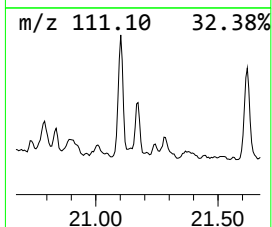
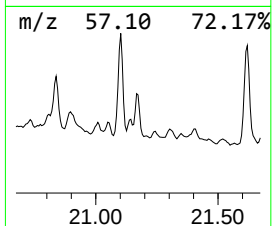
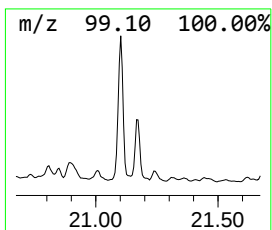
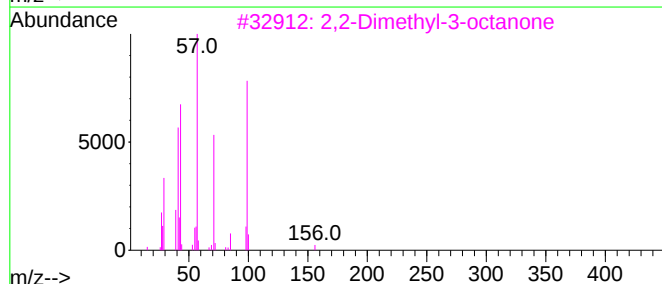
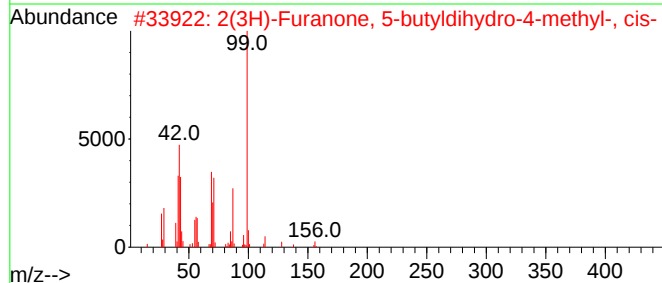
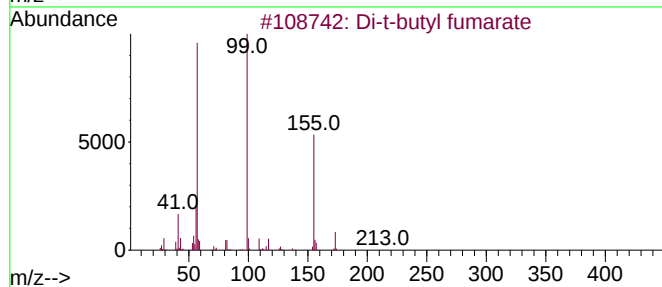
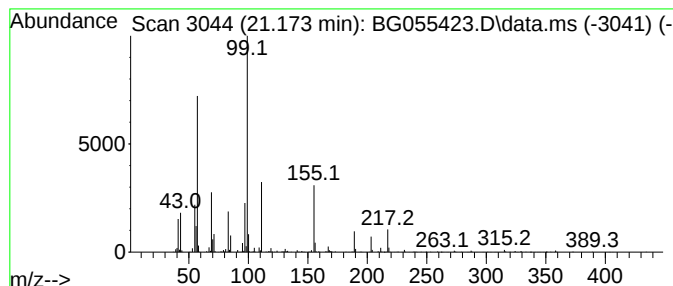
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown21.173 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.173	19.07 ng	1387950	Chrysene-d12	21.872

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-t-butyl fumarate	228	C12H20O4	007633-38-7	38
2			2(3H)-Furanone, 5-butyldihydro-4...	156	C9H16O2	055013-32-6	32
3			2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	32
4			1-Isobutyl-3-methylbutyl methylp...	224	C10H22FO2P	193090-16-3	28
5			D-Gulonic acid, .gamma.-lactone,...	254	C10H16B2O6	074128-60-2	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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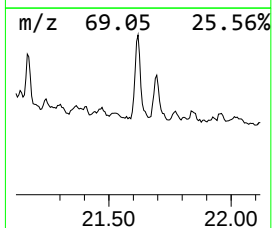
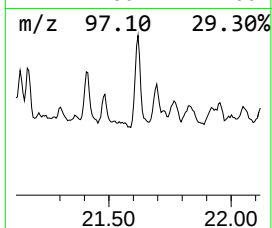
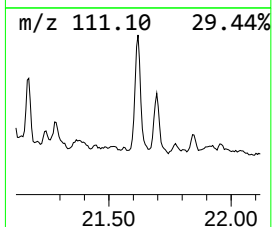
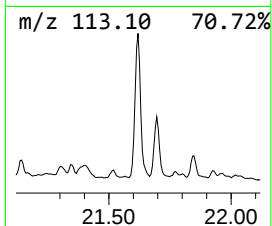
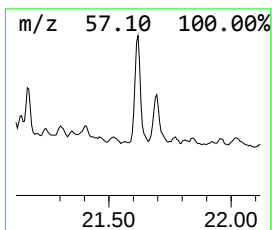
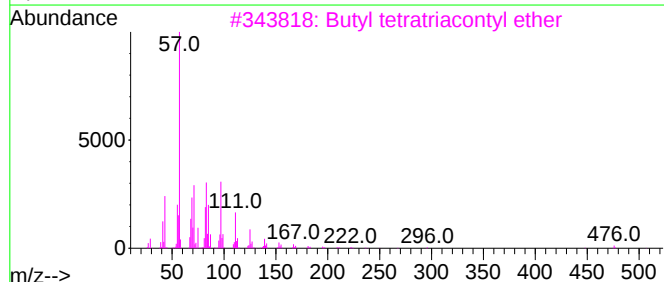
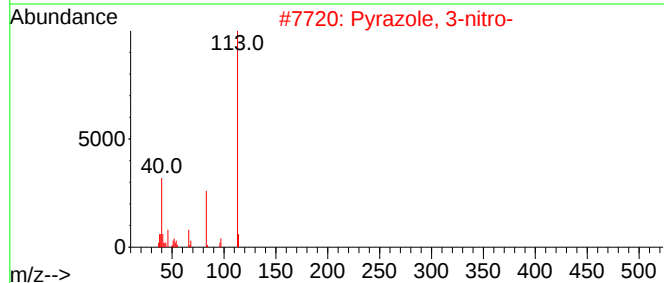
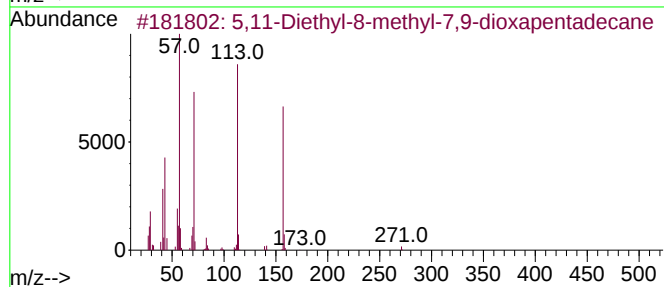
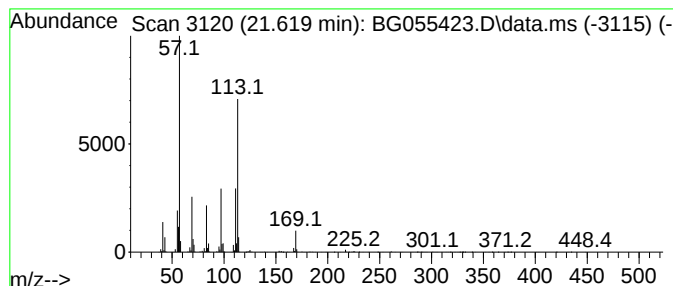
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown21.619 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.619	29.39 ng	2139660	Chrysene-d12	21.872

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,11-Diethyl-8-methyl-7,9-dioxap...	286	C18H38O2	1000334-83-1	32	
2	Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	25	
3	Butyl tetraatriacontyl ether	551	C38H78O	1000406-41-4	25	
4	Ribitol, 1,3:4,5-di-O-(ethylbora...	212	C9H18B2O4	1000149-52-8	25	
5	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	25	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
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Acq On : 2 Nov 2022 20:32
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Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

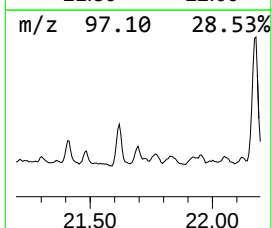
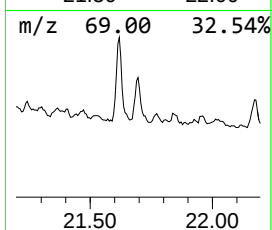
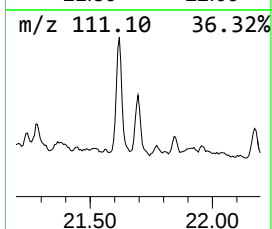
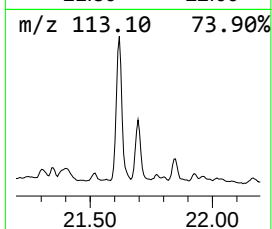
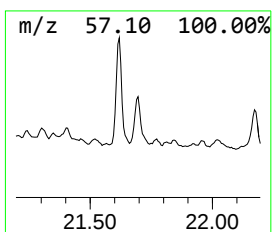
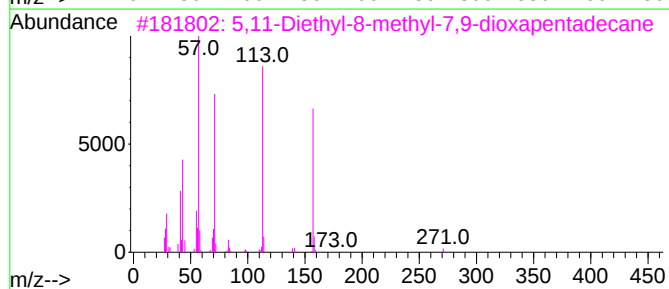
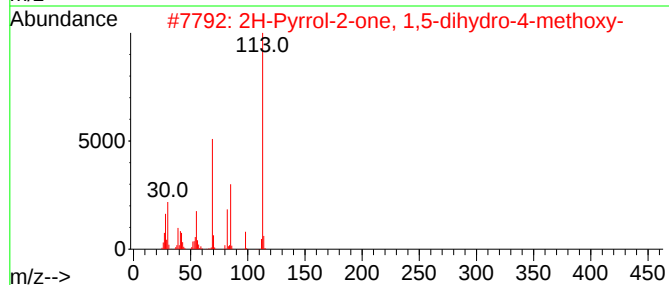
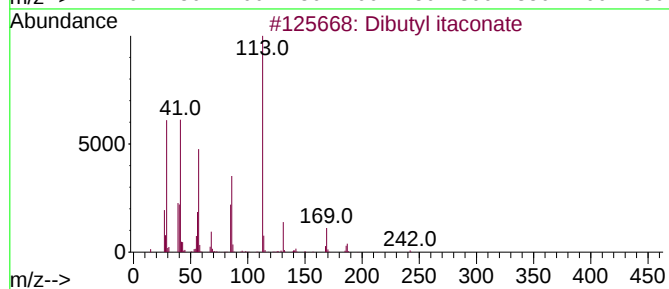
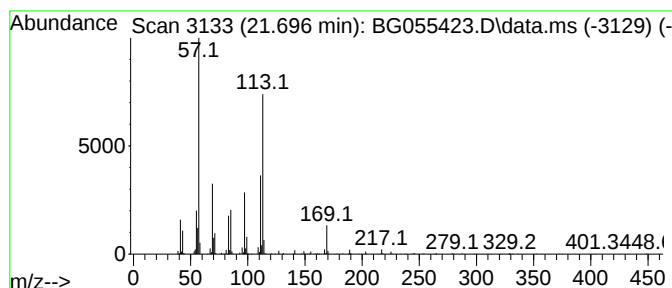
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Dibutyl itaconate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.696	20.00 ng	1455980	Chrysene-d12	21.872	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibutyl itaconate	242	C13H22O4	002155-60-4	50
2	2H-Pyrrol-2-one, 1,5-dihydro-4-m...	113	C5H7NO2	069778-83-2	46
3	5,11-Diethyl-8-methyl-7,9-dioxap...	286	C18H38O2	1000334-83-1	43
4	Borinic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	43
5	Ethosuximide	141	C7H11NO2	000077-67-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

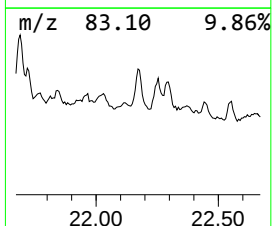
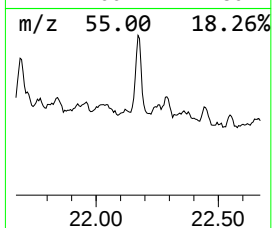
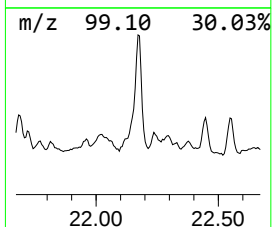
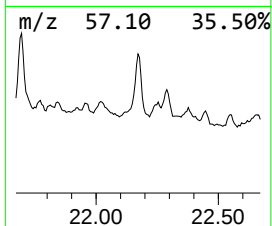
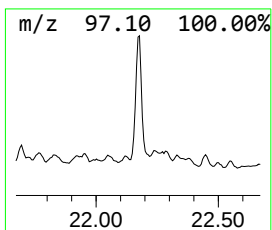
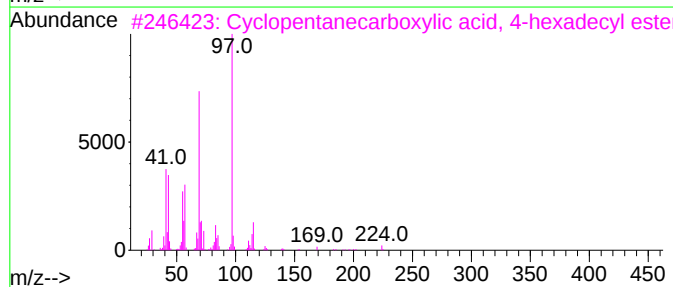
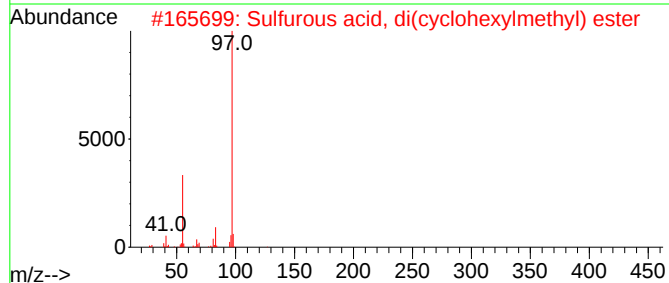
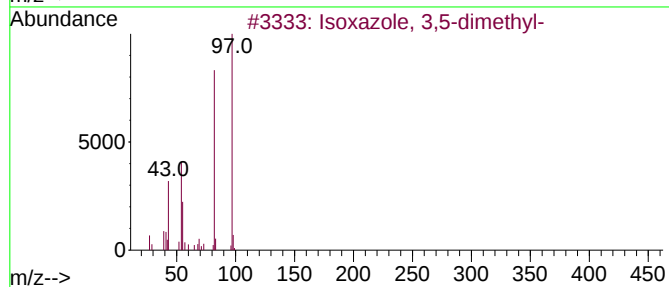
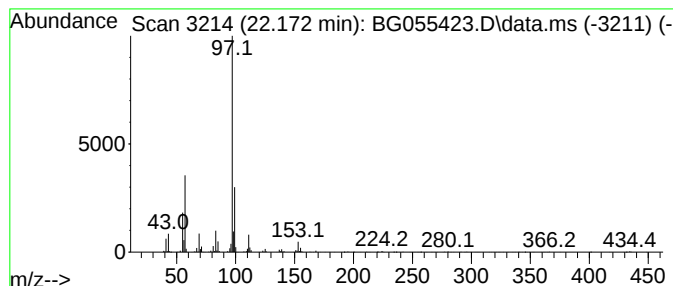
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Sulfurous acid, di(cyclohex... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.172	20.82 ng	1515360	Chrysene-d12		21.872	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Isoxazole, 3,5-dimethyl-		97	C5H7NO	000300-87-8	53
2	Sulfurous acid, di(cyclohexylmet...		274	C14H26O3S	1010309-22-7	50
3	Cyclopentanecarboxylic acid, 4-h...		338	C22H42O2	1000282-77-5	50
4	Thiophene, 2-hexyl-		168	C10H16S	018794-77-9	42
5	Thiophene, 2-decyl-		224	C14H24S	024769-39-9	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

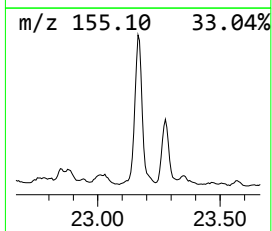
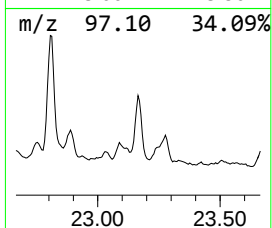
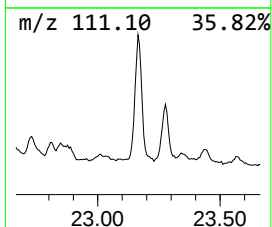
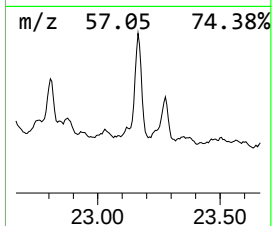
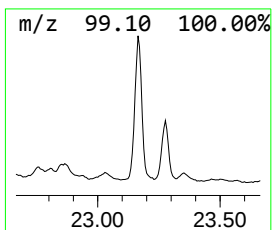
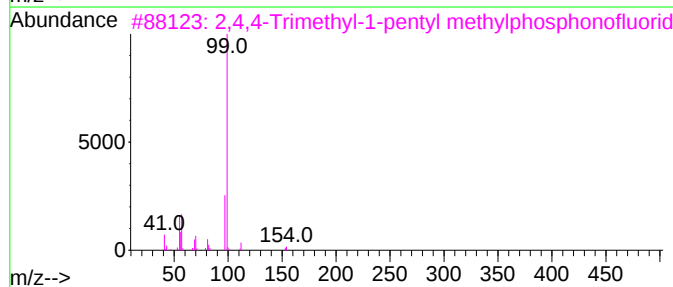
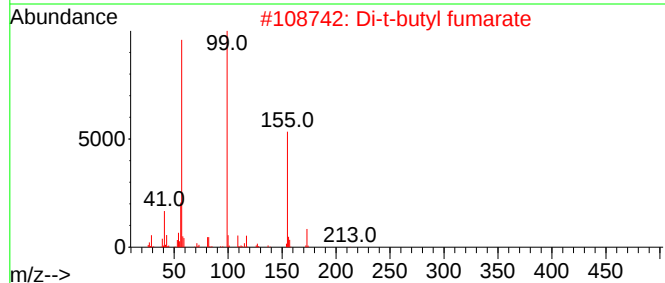
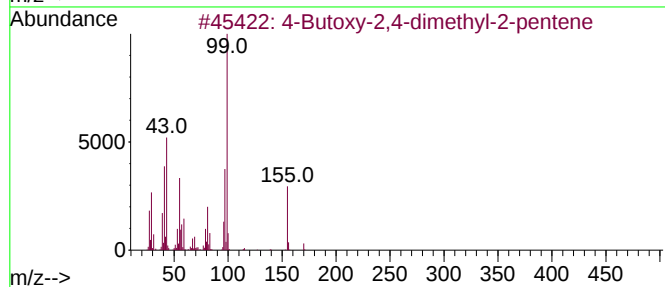
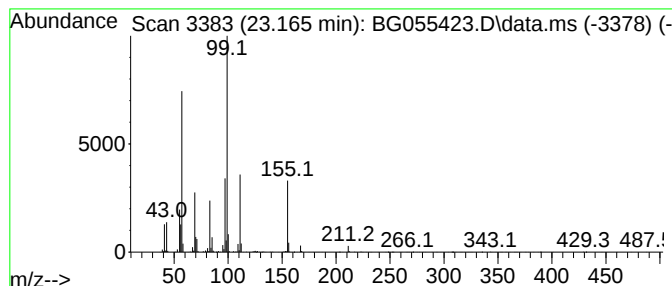
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Di-t-butyl fumarate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.165	36.39 ng	2649260	Chrysene-d12	21.872	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	53
2	Di-t-butyl fumarate	228	C12H20O4	007633-38-7	50
3	2,4,4-Trimethyl-1-pentyl methylp...	210	C9H20F02P	333416-06-1	43
4	Alpinal diethyl acetal	216	C13H28O2	1000430-79-8	40
5	Phosphite, tris(2,4-dimethylpent...	376	C21H45O3P	1000159-84-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20071

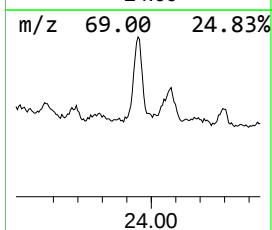
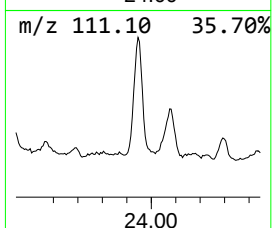
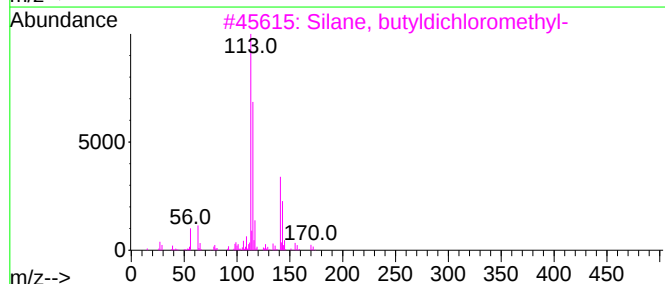
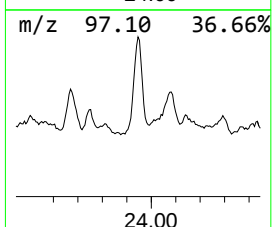
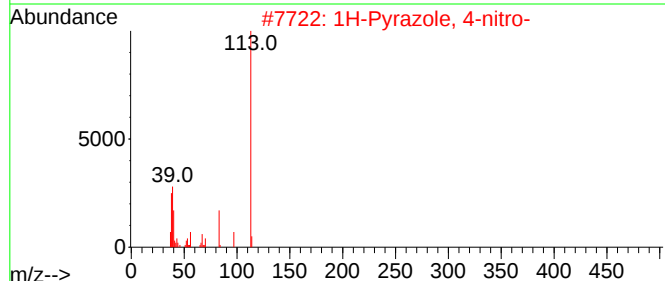
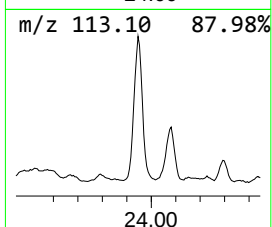
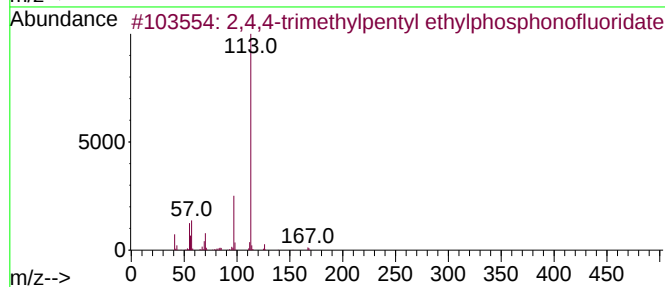
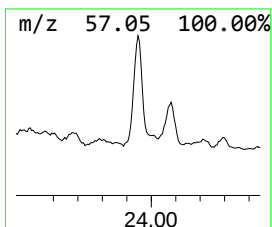
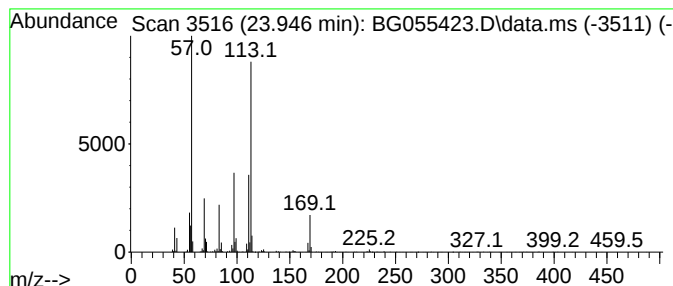
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown23.946 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.946	20.00 ng	1638780	Perylene-d12	25.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4,4-trimethylpentyl ethylphosp...	224	C10H22FO2P	333416-13-0	47
2			1H-Pyrazole, 4-nitro-	113	C3H3N3O2	002075-46-9	43
3			Silane, butyldichloromethyl-	170	C5H12Cl2Si	018147-23-4	38
4			Borinic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	38
5			.beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B2O7	1000156-76-8	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055423.D
Acq On : 2 Nov 2022 20:32
Operator : CG/JU
Sample : N5204-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20071

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.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
unknown7.812	7.812	14.2	ng	138563	1	8.241	195509	20.0
1-Decanol, 2-he...	13.893	38.9	ng	1352940	3	14.857	695845	20.0
unknown14.780	14.780	24.0	ng	836337	3	14.857	695845	20.0
2,4,4,6,6,8,8-H...	15.650	15.9	ng	552792	3	14.857	695845	20.0
Isoxazole, 3,5-...	15.762	32.3	ng	1123050	3	14.857	695845	20.0
unknown16.966	16.966	29.8	ng	3373820	4	17.595	2262220	20.0
Cyclopentanecar...	18.358	22.7	ng	2568280	4	17.595	2262220	20.0
Benzene, (1-met...	18.922	16.0	ng	1810160	4	17.595	2262220	20.0
unknown19.299	19.299	27.1	ng	3060550	4	17.595	2262220	20.0
unknown19.363	19.363	12.6	ng	1427830	4	17.595	2262220	20.0
unknown19.833	19.833	28.8	ng	2098930	5	21.872	1455980	20.0
Cyclohexane, 1,...	20.356	20.6	ng	1499290	5	21.872	1455980	20.0
7-Ethyl-4-tride...	20.838	17.4	ng	1266100	5	21.872	1455980	20.0
4-Butoxy-2,4-di...	21.102	33.2	ng	2415110	5	21.872	1455980	20.0
unknown21.173	21.173	19.1	ng	1387950	5	21.872	1455980	20.0
unknown21.619	21.619	29.4	ng	2139660	5	21.872	1455980	20.0
Dibutyl itaconate	21.696	20.0	ng	1455980	5	21.872	1455980	20.0
Sulfurous acid,...	22.172	20.8	ng	1515360	5	21.872	1455980	20.0
Di-t-butyl fuma...	23.165	36.4	ng	2649260	5	21.872	1455980	20.0
unknown23.946	23.946	20.0	ng	1638780	6	25.256	1638780	20.0