

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
 Data File : BG048713.D
 Acq On : 15 Apr 2021 17:44
 Operator : CG/JU
 Sample : M1998-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-5A

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-BG041421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048713.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.159	305	310	317	rBV2	36024	54237	4.41%	0.494%
2	5.641	384	392	401	rBV	452853	736032	59.89%	6.699%
3	7.256	654	667	668	rBV	531812	947567	77.11%	8.625%
4	7.280	669	671	681	rVB	641773	888734	72.32%	8.089%
5	7.703	739	743	751	rVB3	7954	14750	1.20%	0.134%
6	7.861	765	770	776	rBV6	8202	15922	1.30%	0.145%
7	8.085	798	808	813	rBV	114160	205856	16.75%	1.874%
8	8.138	813	817	825	rVB2	75720	116060	9.44%	1.056%
9	9.260	1001	1008	1015	rBV	372152	642723	52.30%	5.850%
10	9.659	1068	1076	1082	rVB6	12165	22775	1.85%	0.207%
11	10.676	1231	1249	1255	rBV2	203485	731690	59.54%	6.660%
12	10.870	1276	1282	1283	rBV3	10883	14328	1.17%	0.130%
13	10.911	1283	1289	1295	rVB	146385	259958	21.15%	2.366%
14	11.058	1305	1314	1319	rBV5	10530	22193	1.81%	0.202%
15	11.816	1439	1443	1451	rVB8	7089	13575	1.10%	0.124%
16	11.921	1457	1461	1464	rBV5	13941	19335	1.57%	0.176%
17	12.010	1473	1476	1483	rVB7	7841	16613	1.35%	0.151%
18	12.104	1487	1492	1498	rBV8	9057	19426	1.58%	0.177%
19	12.409	1535	1544	1552	rBV	258151	439291	35.75%	3.998%
20	12.644	1580	1584	1590	rVB6	16491	30785	2.51%	0.280%
21	12.938	1630	1634	1641	rBV9	7753	16865	1.37%	0.154%
22	13.261	1684	1689	1692	rVV4	17160	22225	1.81%	0.202%
23	13.361	1696	1706	1715	rVB	758936	1188610	96.72%	10.819%
24	13.525	1728	1734	1736	rBV5	12353	22118	1.80%	0.201%
25	13.549	1736	1738	1745	rVB6	18604	42080	3.42%	0.383%
26	13.649	1750	1755	1761	rVV4	20033	29015	2.36%	0.264%
27	14.107	1832	1833	1838	rVB5	11006	12440	1.01%	0.113%
28	14.160	1838	1842	1843	rBV3	25552	30329	2.47%	0.276%
29	14.313	1864	1868	1874	rVB6	17829	29505	2.40%	0.269%
30	14.477	1890	1896	1901	rBV9	12017	27944	2.27%	0.254%
31	14.577	1908	1913	1917	rBV7	20733	39445	3.21%	0.359%
32	14.701	1930	1934	1935	rBV4	14375	18192	1.48%	0.166%
33	14.742	1935	1941	1948	rVB2	207572	346001	28.16%	3.149%
34	15.129	2002	2007	2011	rBV8	13531	25964	2.11%	0.236%
35	15.223	2019	2023	2031	rVB8	17568	41123	3.35%	0.374%
36	15.529	2070	2075	2079	rBV8	19422	39121	3.18%	0.356%

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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

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37	15.570	2080	2082	2086	rVB5	18973	17430	1.42%	0.159%
38	15.735	2107	2110	2114	rBV4	12937	19048	1.55%	0.173%
39	15.981	2148	2152	2156	rVB6	20622	34351	2.80%	0.313%
40	16.234	2190	2195	2202	rVB2	145629	216602	17.63%	1.971%
41	16.457	2227	2233	2240	rVB5	56853	112808	9.18%	1.027%
42	16.563	2247	2251	2254	rBV2	26211	37633	3.06%	0.343%
43	16.686	2268	2272	2275	rBV6	21982	29776	2.42%	0.271%
44	16.880	2301	2305	2306	rBV4	29377	36322	2.96%	0.331%
45	16.951	2314	2317	2321	rVB3	16878	22796	1.85%	0.207%
46	17.010	2321	2327	2334	rBV10	31365	74025	6.02%	0.674%
47	17.250	2360	2368	2372	rBV3	125807	228536	18.60%	2.080%
48	17.497	2405	2410	2415	rBV	238553	356600	29.02%	3.246%
49	17.562	2419	2421	2426	rVB3	56719	77746	6.33%	0.708%
50	17.744	2450	2452	2456	rVB4	20070	19183	1.56%	0.175%
51	17.891	2475	2477	2479	rBV3	14390	14446	1.18%	0.131%
52	18.379	2556	2560	2564	rBV6	50806	72294	5.88%	0.658%
53	18.426	2566	2568	2571	rVB4	21025	21721	1.77%	0.198%
54	18.537	2583	2587	2591	rVB	92522	118175	9.62%	1.076%
55	19.389	2729	2732	2736	rBV3	48752	57231	4.66%	0.521%
56	19.565	2758	2762	2766	rBV	56092	71940	5.85%	0.655%
57	19.918	2819	2822	2826	rVB	62518	83919	6.83%	0.764%
58	20.112	2850	2855	2859	rVB	981180	1228899	100.00%	11.185%
59	21.416	3073	3077	3082	rVB3	100582	133401	10.86%	1.214%
60	21.669	3116	3120	3124	rVB3	86615	116308	9.46%	1.059%
61	21.798	3137	3142	3148	rVB	197508	345945	28.15%	3.149%
62	25.147	3707	3712	3721	rVB2	108169	283942	23.11%	2.584%
63	28.813	4334	4336	4339	rVB4	14803	12761	1.04%	0.116%

Sum of corrected areas: 10986665

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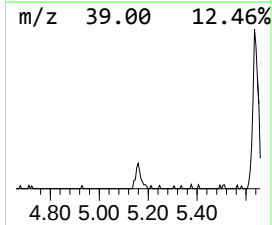
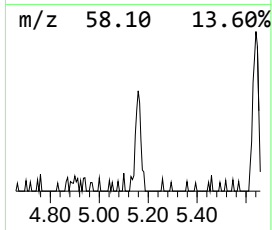
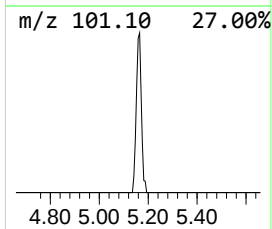
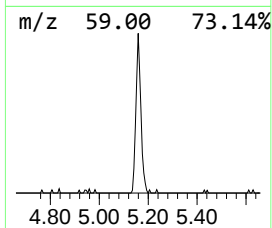
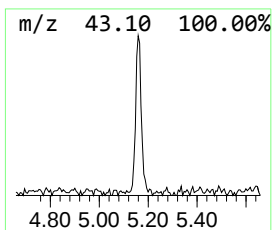
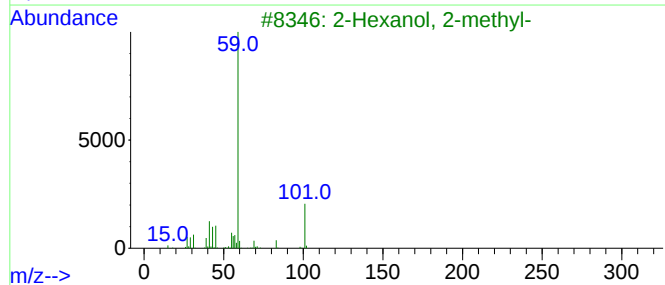
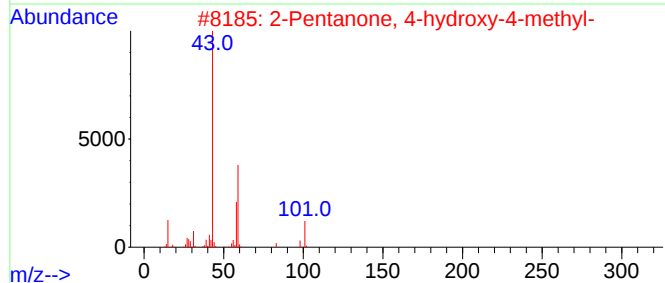
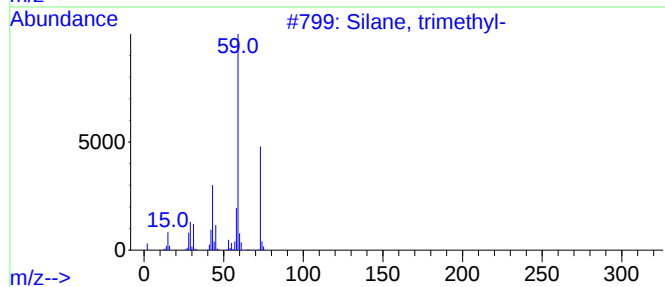
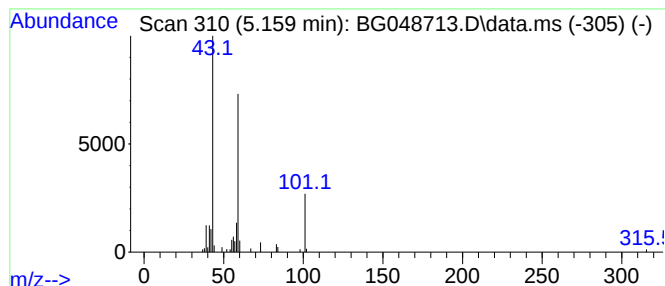
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown5.159 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.159	5.27 ng	54237	1,4-Dichlorobenzene-d4	8.085

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silane, trimethyl-	74	C3H10Si	000993-07-7	42
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	36
5			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36



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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
SB-5A

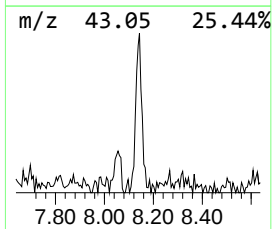
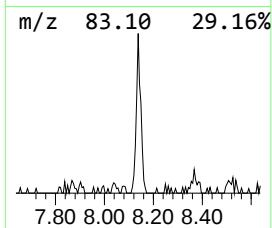
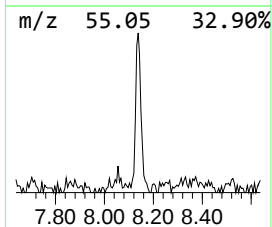
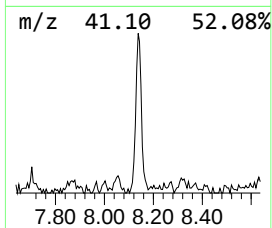
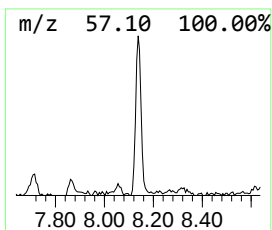
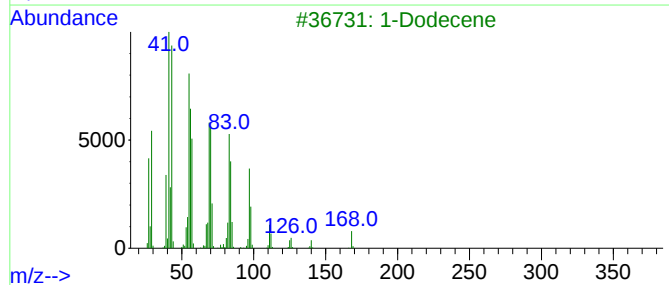
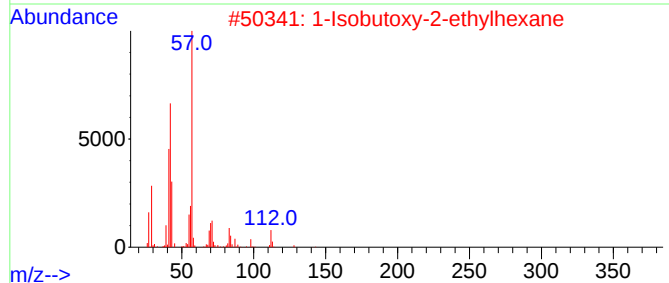
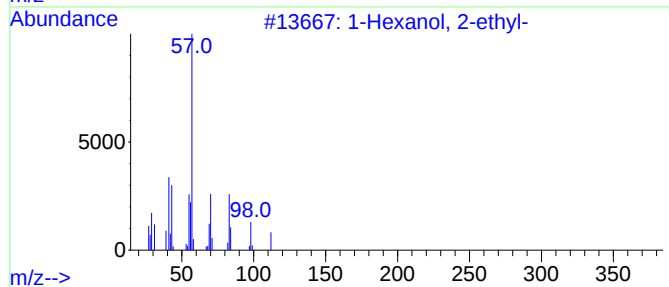
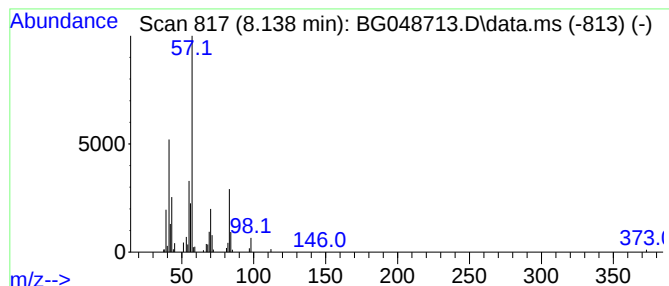
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.138	11.28 ng	116060	1,4-Dichlorobenzene-d4	8.085

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	64
3			1-Dodecene	168	C12H24	000112-41-4	47
4			1-Undecene	154	C11H22	000821-95-4	47
5			2-Tridecene, (Z)-	182	C13H26	041446-59-7	47



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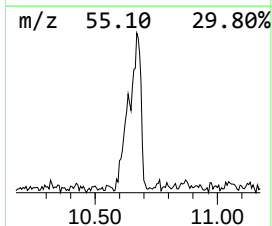
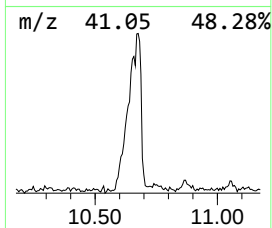
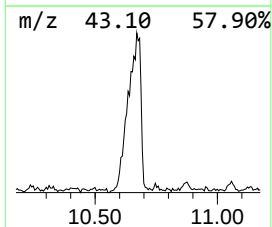
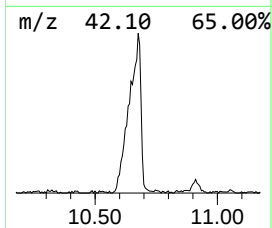
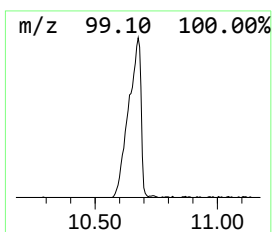
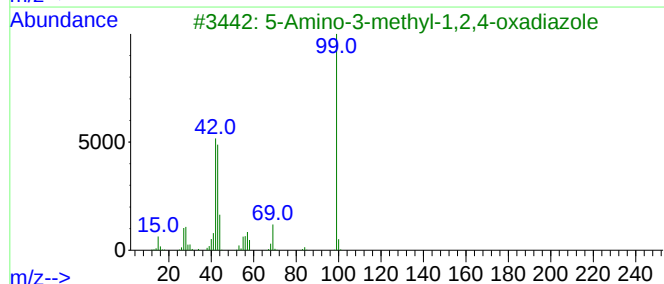
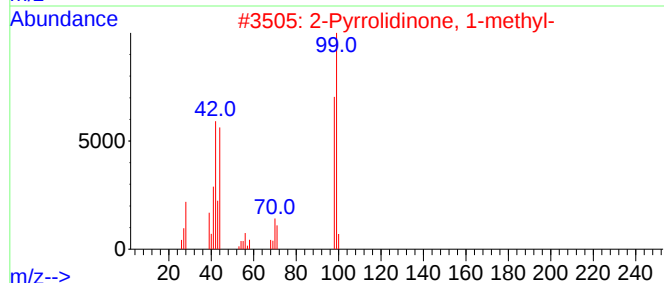
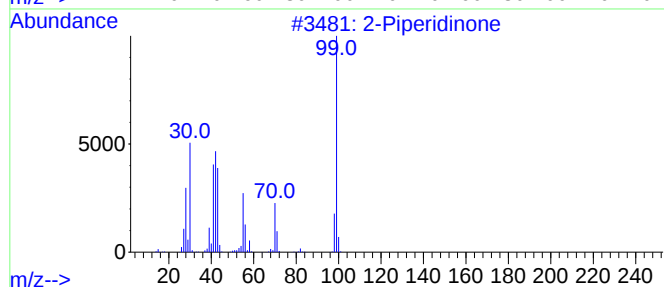
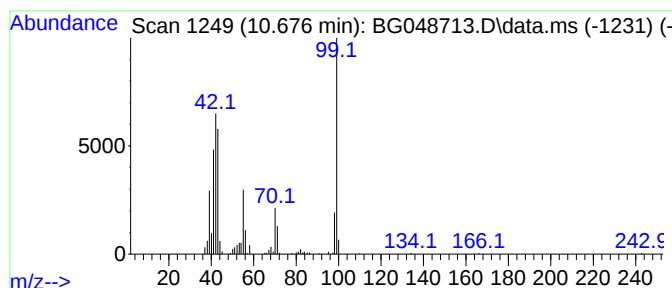
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Piperidinone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.676	56.29 ng	731690	Naphthalene-d8	10.911

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Piperidinone	99	C5H9NO	000675-20-7	87
2			2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	72
3			5-Amino-3-methyl-1,2,4-oxadiazole	99	C3H5N3O	003663-39-6	53
4			Piperidine-4,4-diol	117	C5H11NO2	1000302-71-5	50
5			Thiazole, 5-methyl-	99	C4H5NS	003581-89-3	47



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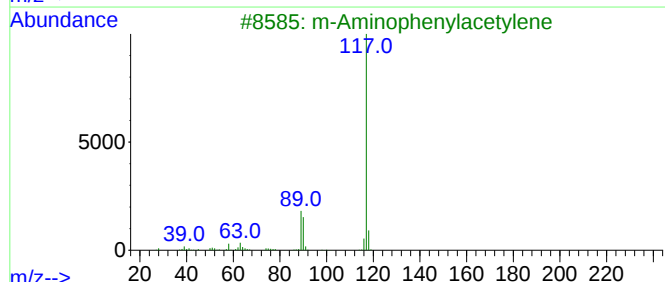
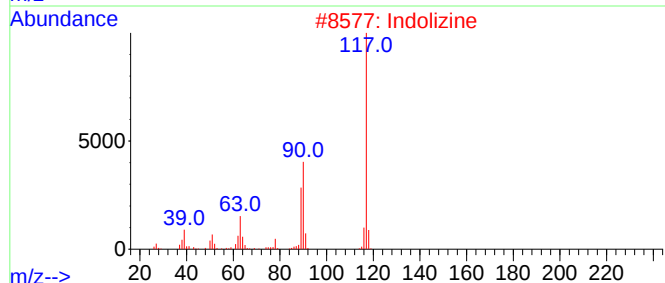
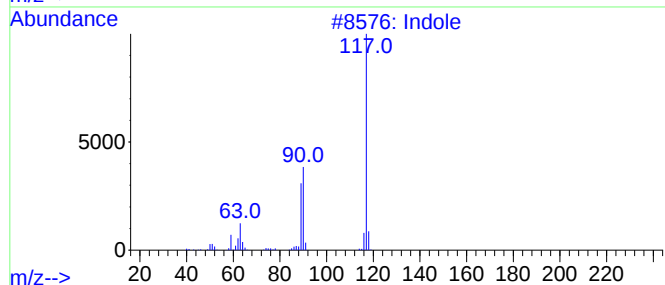
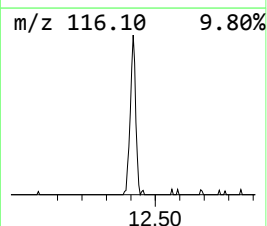
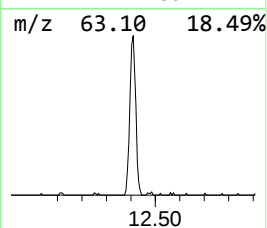
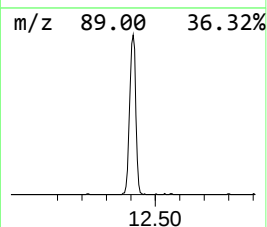
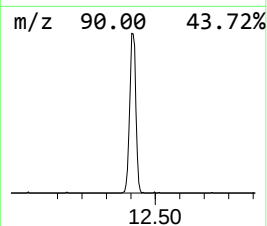
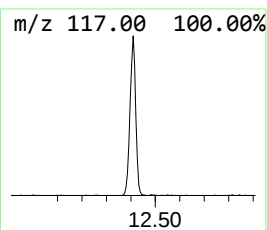
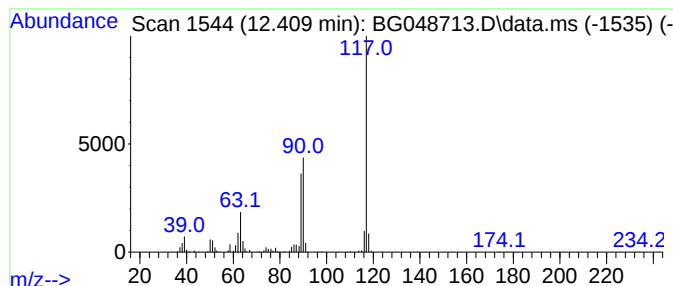
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Indole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.409	33.80 ng	439291	Naphthalene-d8	10.911

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	95
2			Indolizine	117	C8H7N	000274-40-8	91
3			m-Aminophenylacetylene	117	C8H7N	054060-30-9	90
4			Benzyl nitrile	117	C8H7N	000140-29-4	87
5			Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	86



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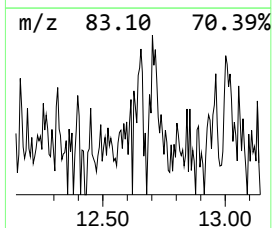
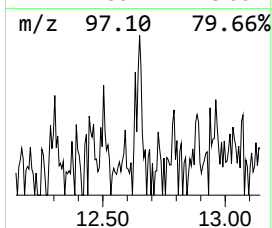
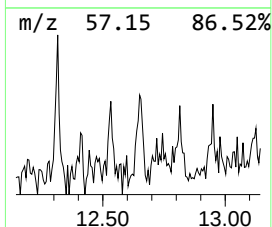
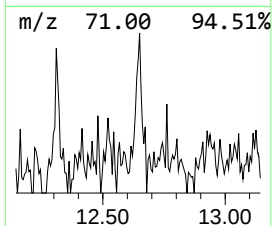
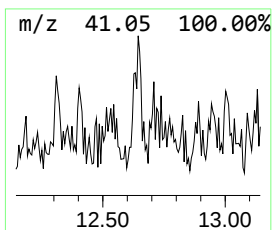
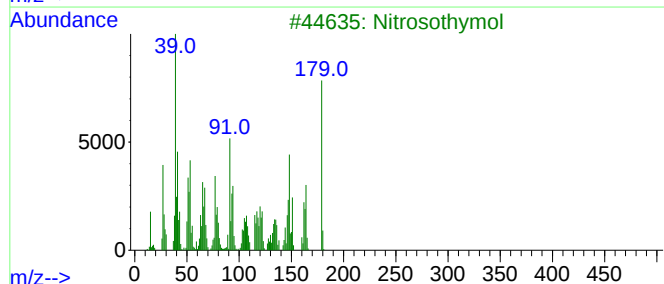
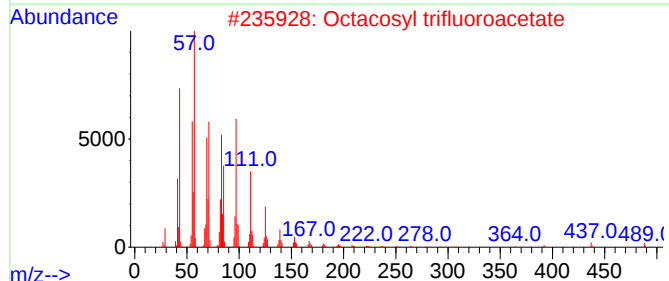
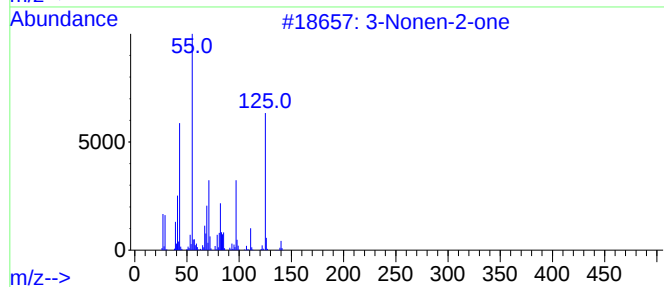
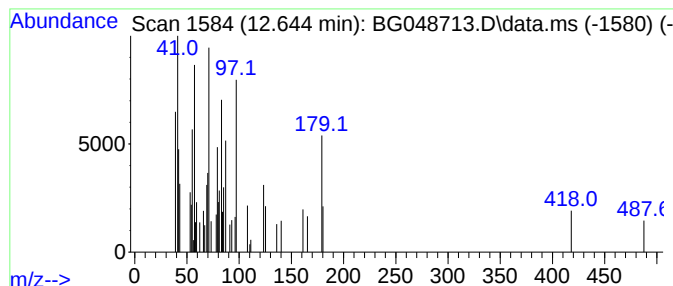
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown12.644 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.644	2.37 ng	30785	Naphthalene-d8	10.911

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Nonen-2-one	140	C9H16O	014309-57-0	22
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	22
3			Nitrosothymol	179	C10H13NO2	002364-54-7	14
4			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	12
5			2-Butenoic acid, 2-cyano-3-methy...	153	C8H11NO2	000759-58-0	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
Operator : CG/JU
Sample : M1998-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-5A

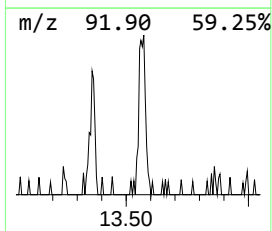
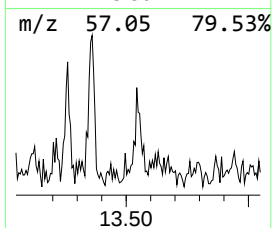
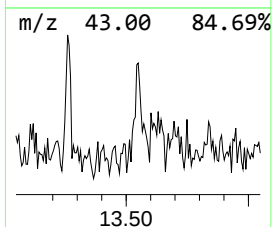
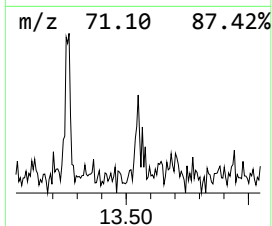
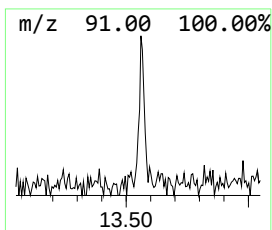
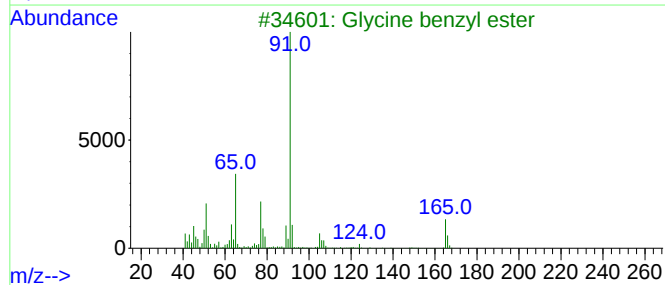
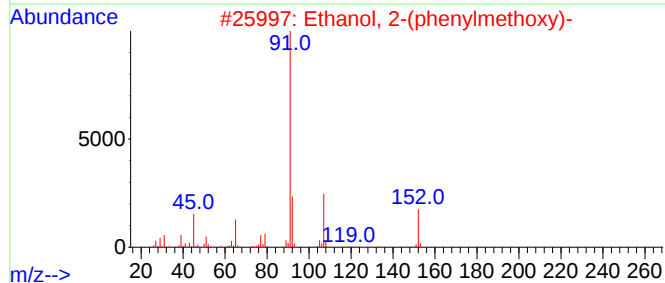
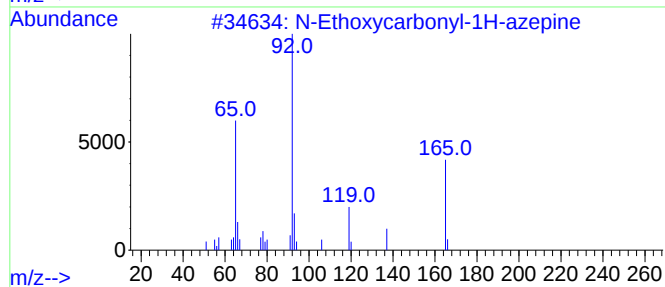
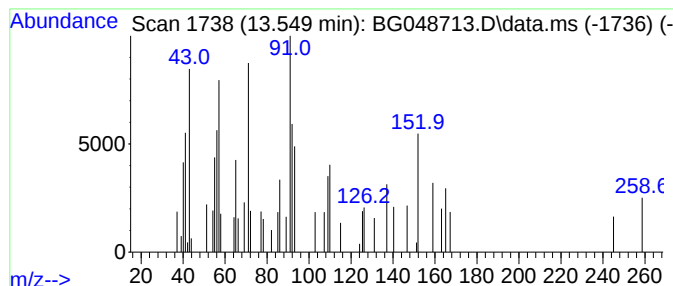
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown13.549 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.549	2.43 ng	42080	Acenaphthene-d10	14.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Ethoxycarbonyl-1H-azepine	165	C9H11NO2	002955-79-5	43
2			Ethanol, 2-(phenylmethoxy)-	152	C9H12O2	000622-08-2	38
3			Glycine benzyl ester	165	C9H11NO2	001738-68-7	35
4			Piperonyl alcohol	152	C8H8O3	000495-76-1	35
5			1,6-Heptadien-3-yne	92	C7H8	005150-80-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
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Sample : M1998-08
Misc :
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Instrument :
BNA_G
ClientSampled :
SB-5A

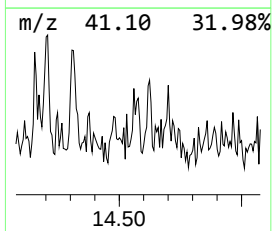
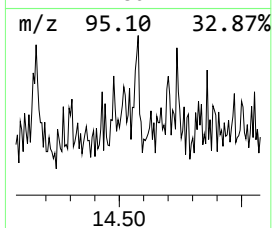
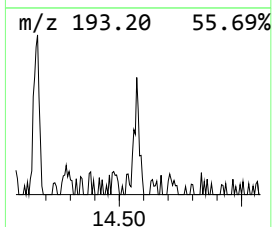
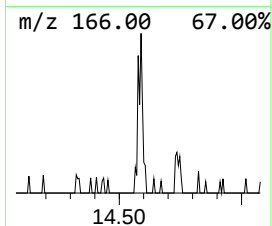
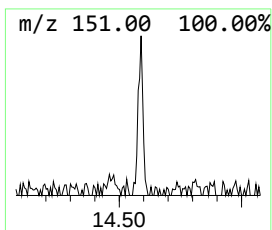
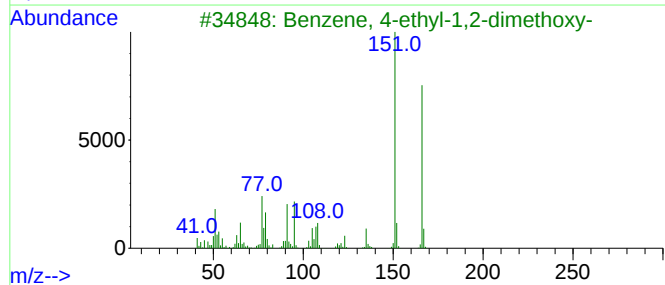
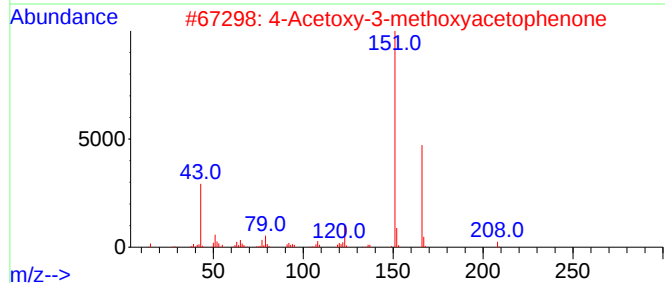
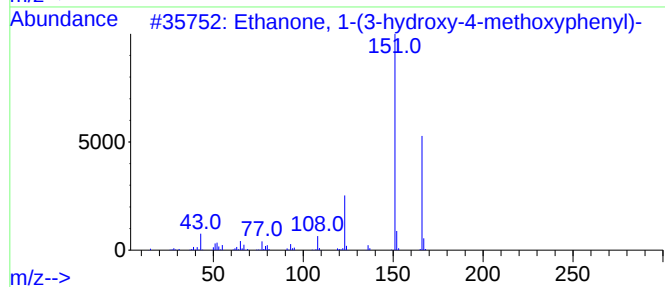
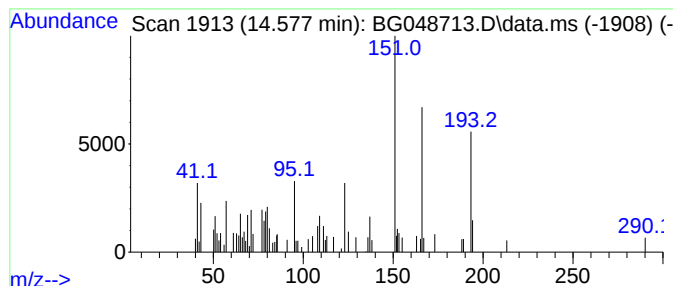
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown14.577 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.577	2.28 ng	39445	Acenaphthene-d10	14.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	49
2			4-Acetoxy-3-methoxyacetophenone	208	C11H12O4	054771-60-7	47
3			Benzene, 4-ethyl-1,2-dimethoxy-	166	C10H14O2	005888-51-7	46
4			1,4-Dimethoxy-2,3-dimethylbenzene	166	C10H14O2	039021-83-5	46
5			Ethanone, 1-(2-hydroxy-4-methoxy...	166	C9H10O3	000552-41-0	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
Operator : CG/JU
Sample : M1998-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
SB-5A

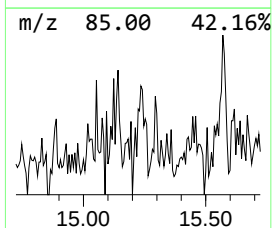
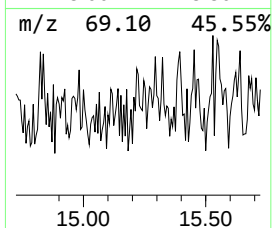
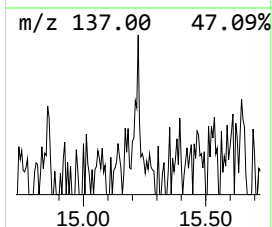
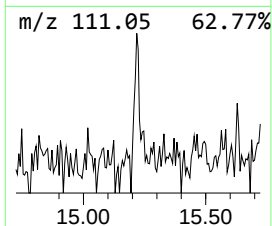
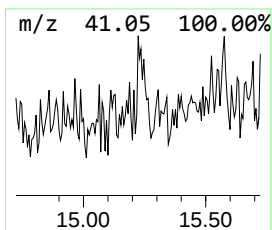
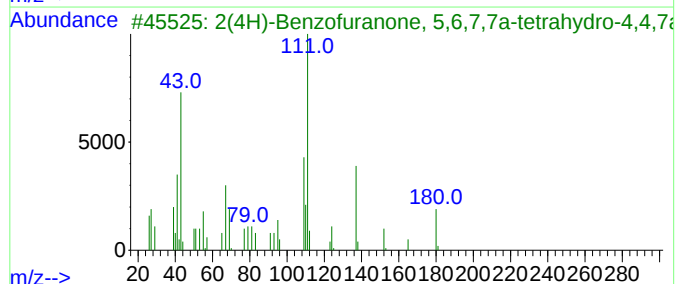
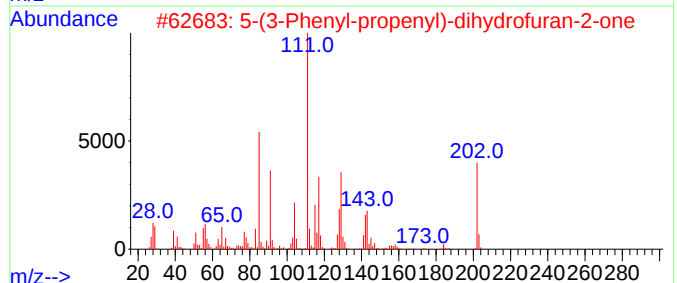
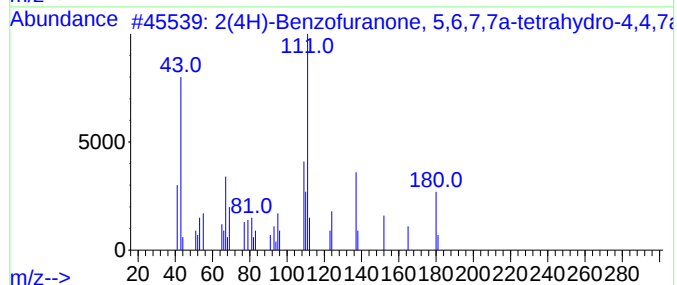
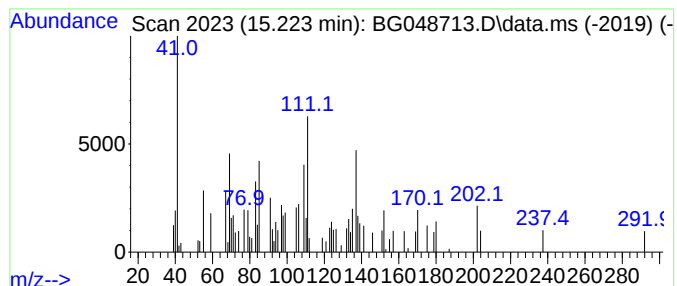
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown15.224 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.224	2.38 ng	41123	Acenaphthene-d10	14.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(4H)-Benzofuranone, 5,6,7,7a-te...	180	C11H16O2	017092-92-1	22		
2	5-(3-Phenyl-propenyl)-dihydrofur...	202	C13H14O2	1000193-62-6	22		
3	2(4H)-Benzofuranone, 5,6,7,7a-te...	180	C11H16O2	015356-74-8	18		
4	1-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-25-7	10		
5	2-Isopropylidene-5-methylhex-4-enal	152	C10H16O	003304-28-7	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
Operator : CG/JU
Sample : M1998-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

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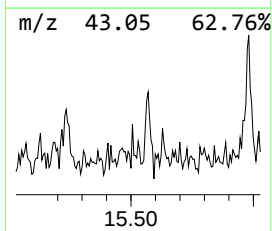
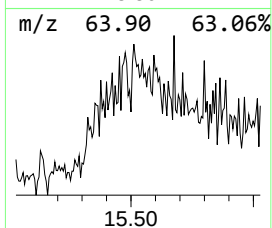
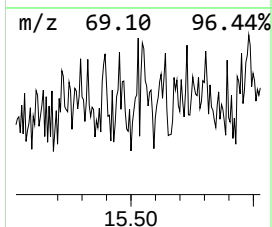
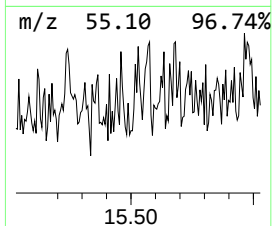
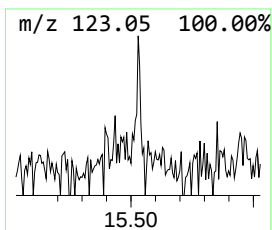
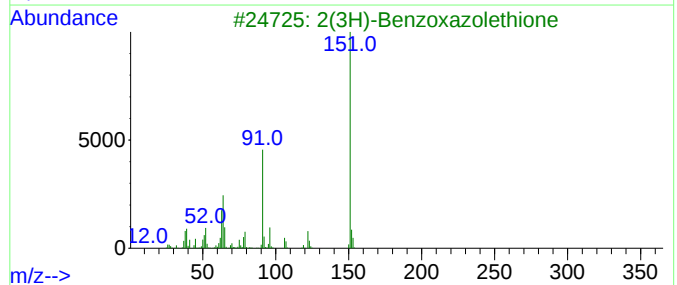
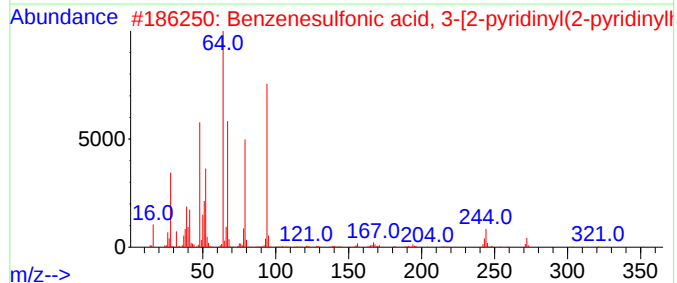
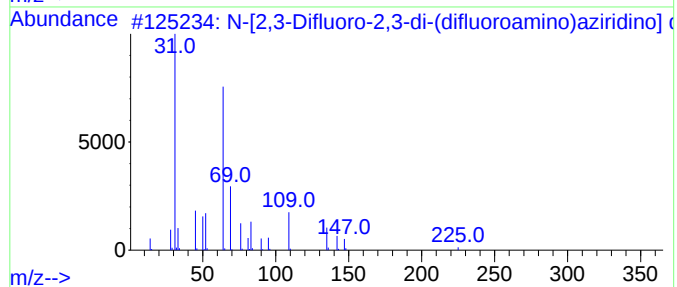
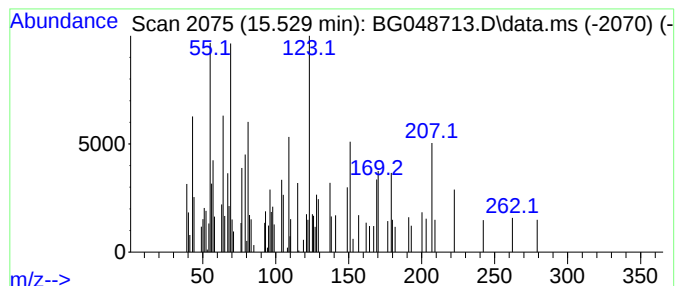
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown15.529 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.529	2.26 ng	39121	Acenaphthene-d10	14.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-[2,3-Difluoro-2,3-di-(difluoro...	277	C3F9N5	1000305-83-6	12
2			Benzenesulfonic acid, 3-[2-pyrid...	354	C17H14N4O3S	052018-85-6	12
3			2(3H)-Benzoxazolethione	151	C7H5NOS	002382-96-9	11
4			benz[d]isoxazole, 4,5,6,7-tetra...	151	C8H9NO2	061834-40-0	11
5			5H-Benzo[b]pyran-8-ol, 2,3,5,5,8...	222	C14H22O2	097306-66-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
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Sample : M1998-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

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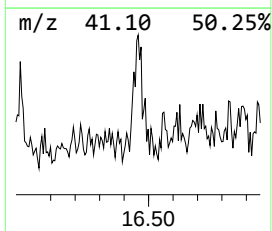
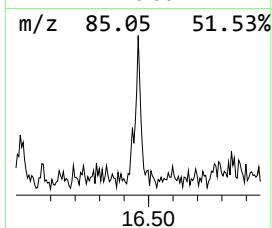
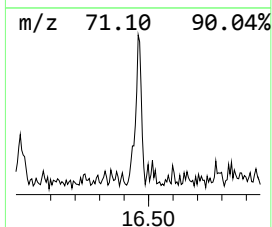
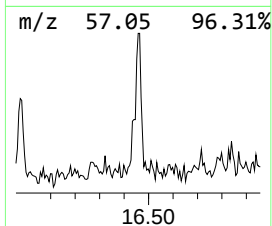
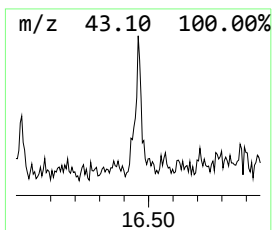
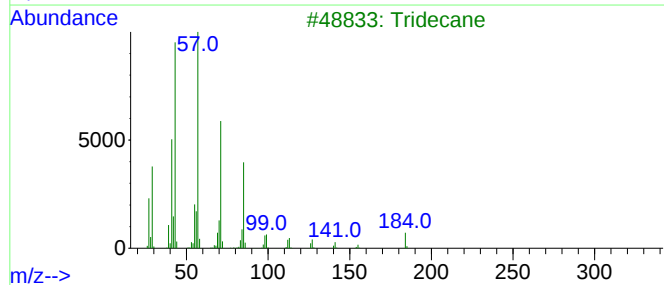
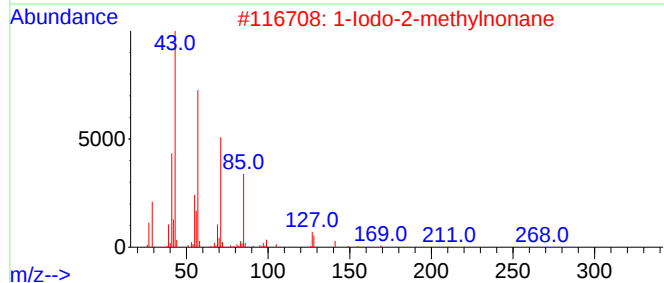
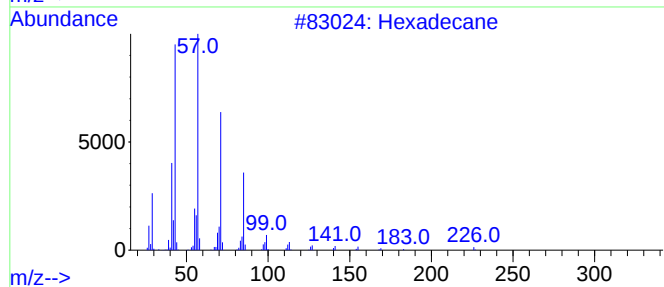
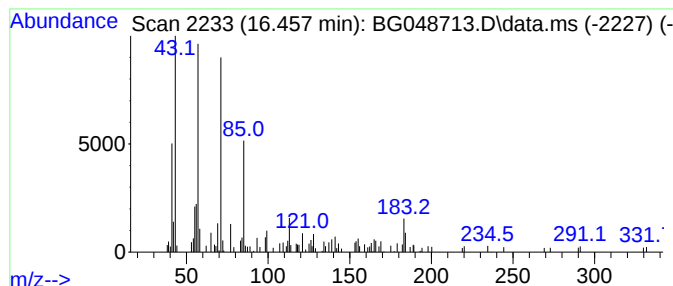
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.457	6.33 ng	112808	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	80
2			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	80
3			Tridecane	184	C13H28	000629-50-5	62
4			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	58
5			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
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Misc :
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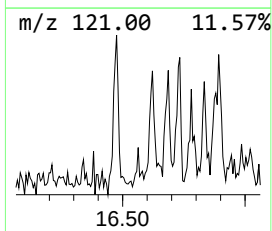
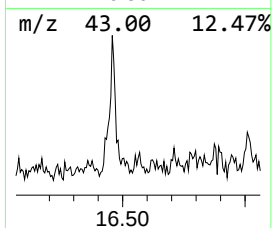
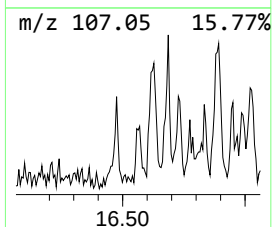
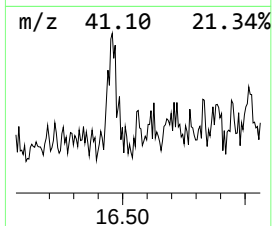
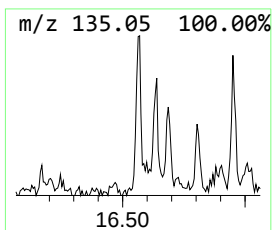
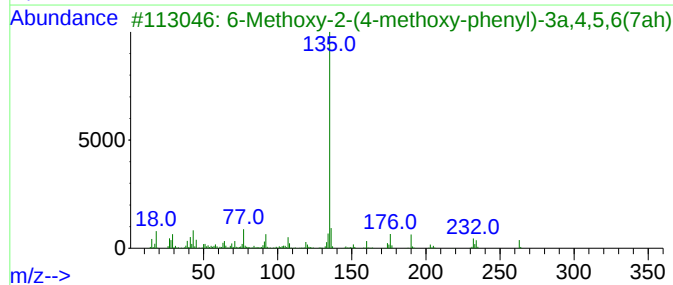
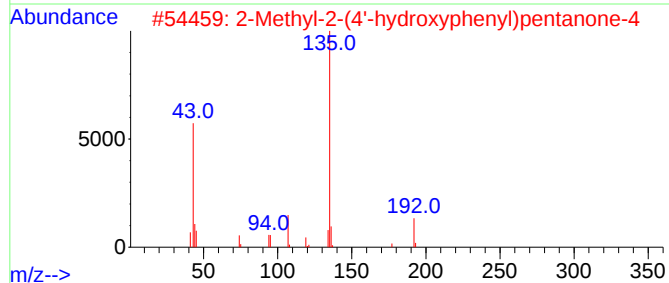
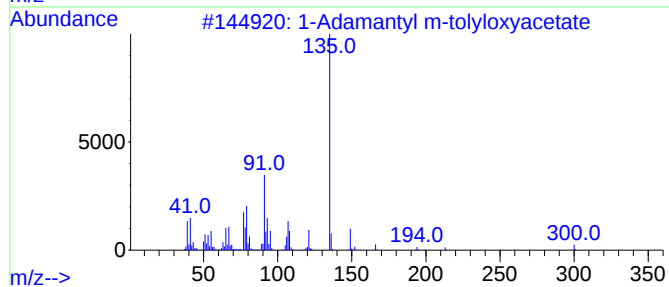
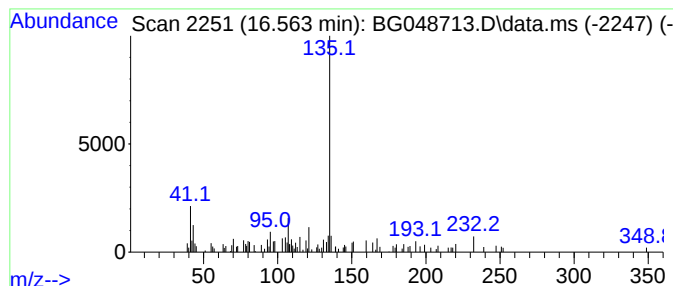
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SB-5A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 1-Adamantyl m-tolyloxyacetate Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.563	2.11 ng	37633	Phenanthrene-d10	17.497		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Adamantyl m-tolyloxyacetate	300	C19H24O3	306278-20-6	72	
2	2-Methyl-2-(4'-hydroxyphenyl)pen...	192	C12H16O2	070205-18-4	59	
3	6-Methoxy-2-(4-methoxy-phenyl)-3...	263	C14H17NO4	1000287-53-8	53	
4	Thymol	150	C10H14O	000089-83-8	53	
5	Aziridinone, 1-(1,1-dimethylethy...	247	C16H25NO	016664-32-7	53	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
Operator : CG/JU
Sample : M1998-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

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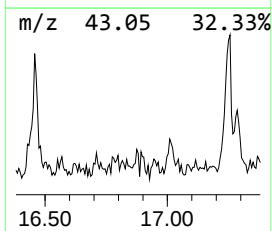
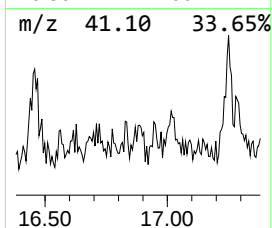
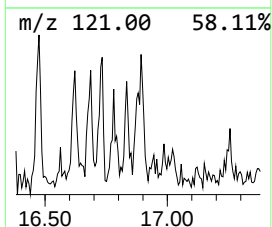
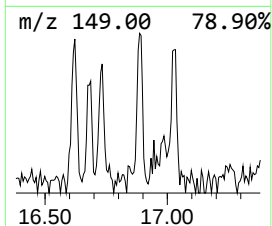
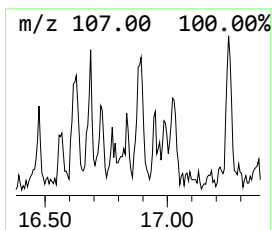
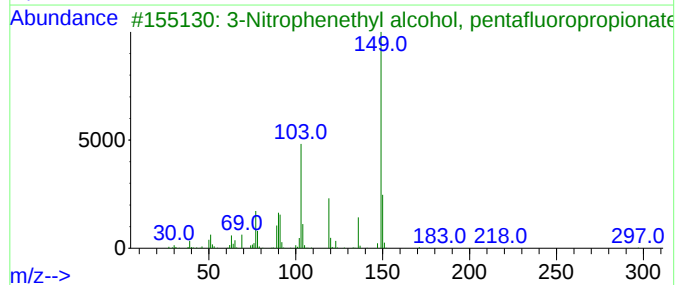
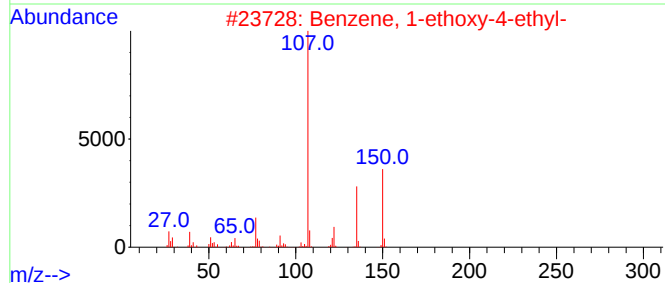
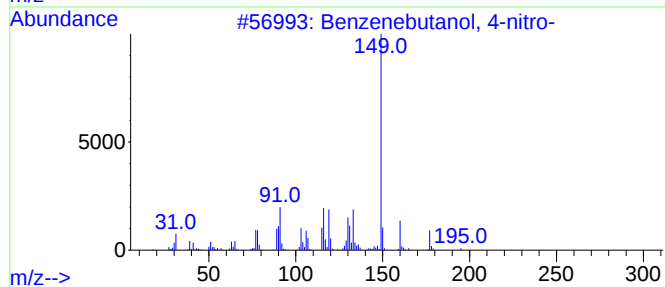
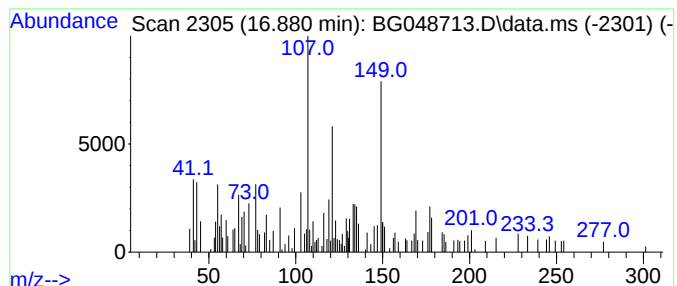
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown16.880 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.880	2.04 ng	36322	Phenanthrene-d10	17.497

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenebutanol, 4-nitro-	195	C10H13NO3	079524-20-2	27
2		Benzene, 1-ethoxy-4-ethyl-	150	C10H14O	001585-06-4	22
3		3-Nitrophenethyl alcohol, pentafluoropropionate	313	C11H8F5NO4	1000364-56-0	22
4		Benzeneamine, 3-hexyl-	177	C12H19N	036042-29-2	22
5		Tricyclo[3.3.1.1(3,7)]decanone, ...	276	C10H13IO	056781-86-3	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
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Sample : M1998-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

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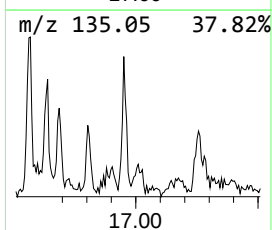
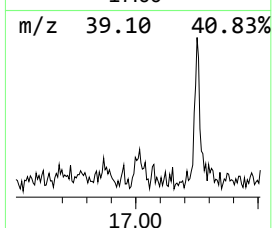
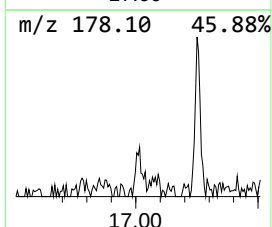
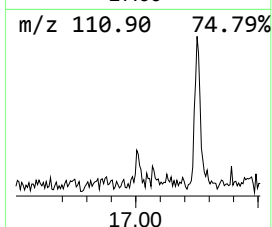
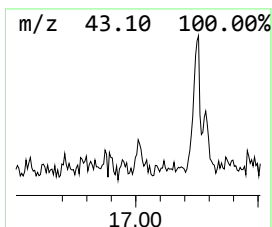
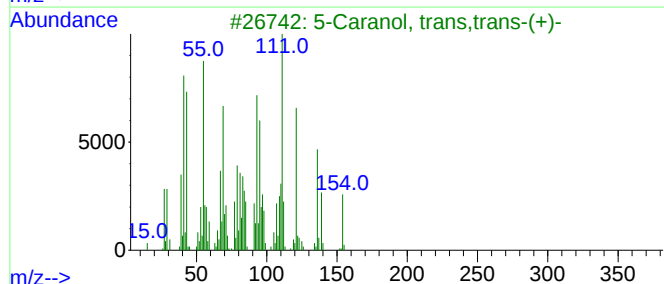
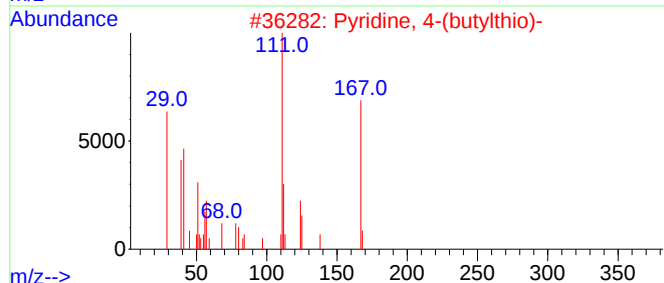
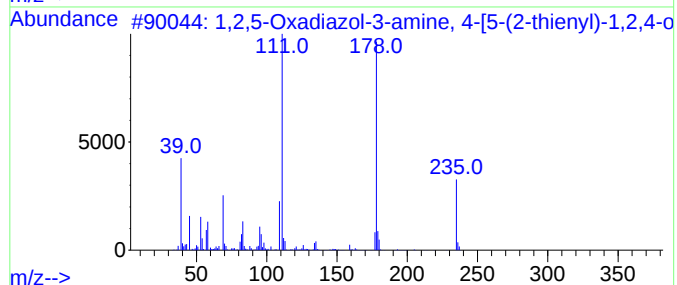
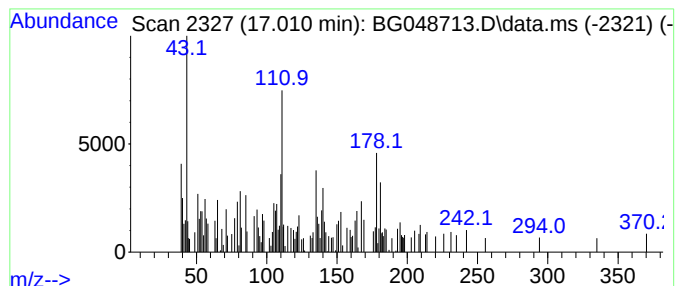
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown17.010 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.010	4.15 ng	74025	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,5-Oxadiazol-3-amine, 4-[5-(2...	235	C8H5N5O2S	1000277-21-2	46		
2	Pyridine, 4-(butylthio)-	167	C9H13NS	026891-64-5	35		
3	5-Caranol, trans,trans-(+)-	154	C10H18O	006909-22-4	35		
4	Cyclopenta-1,3-dioxin-4(5H)-one,...	196	C11H16O3	124899-12-3	30		
5	2-Propenal, 2-methyl-, diethylhy...	140	C8H16N2	075268-11-0	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
Operator : CG/JU
Sample : M1998-08
Misc :
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ClientSampleId :
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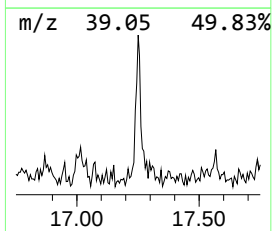
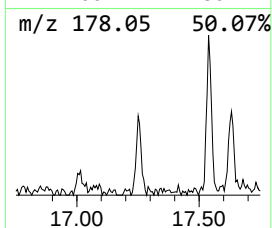
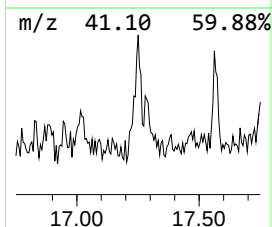
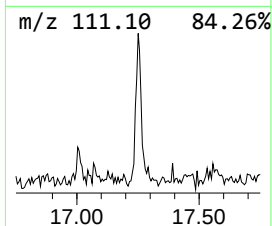
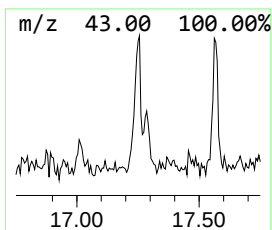
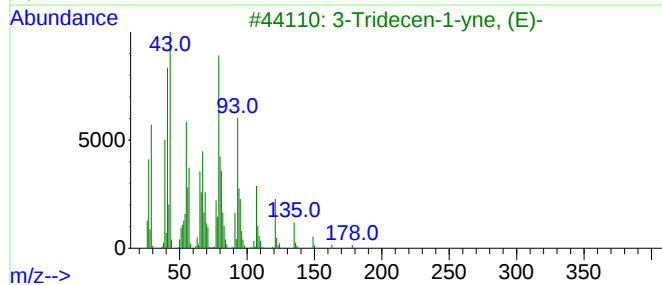
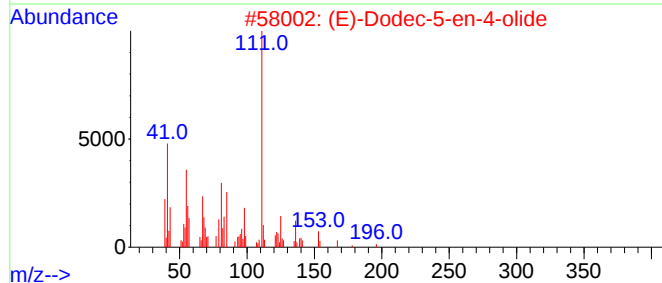
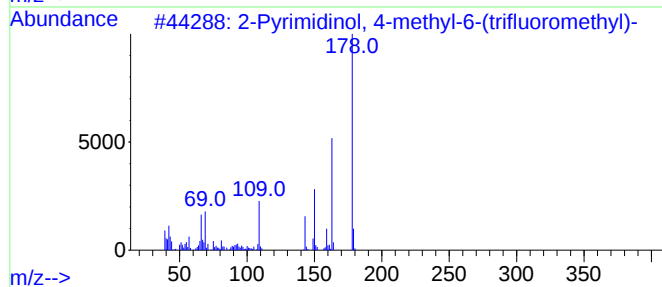
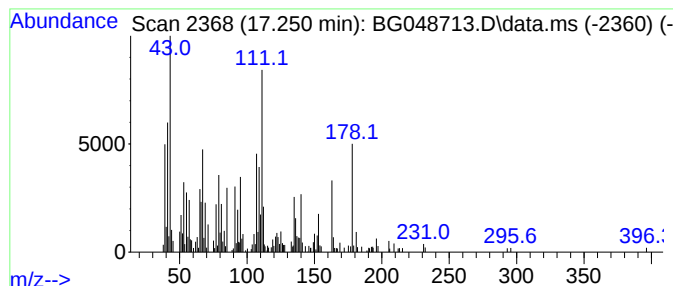
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown17.250 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.250	12.82 ng	228536	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrimidinol, 4-methyl-6-(trifl...	178	C6H5F3N2O	104048-92-2	16		
2	(E)-Dodec-5-en-4-olide	196	C12H20O2	1000370-40-3	15		
3	3-Tridecen-1-yne, (E)-	178	C13H22	074744-41-5	14		
4	Thiophene, 2-methyl-5-propyl-	140	C8H12S	033933-73-2	11		
5	9-Borabicyclo[3.3.1]nonane, 9-(2...	178	C11H19BO	1000162-57-7	11		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
Operator : CG/JU
Sample : M1998-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-5A

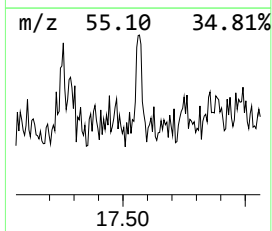
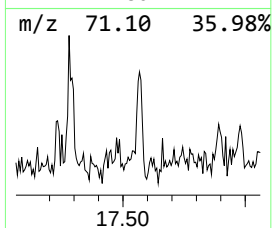
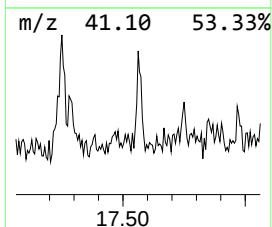
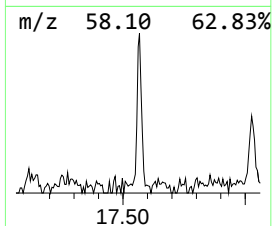
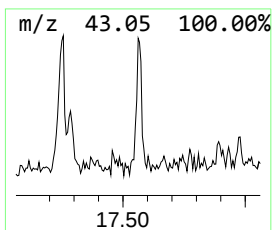
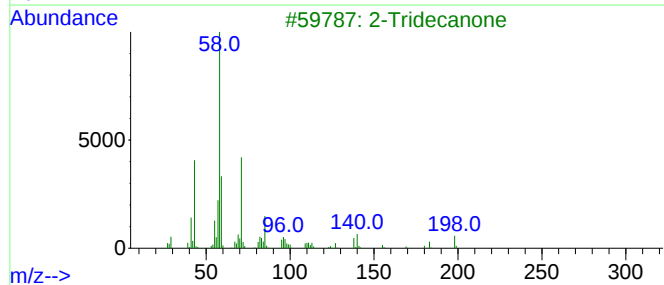
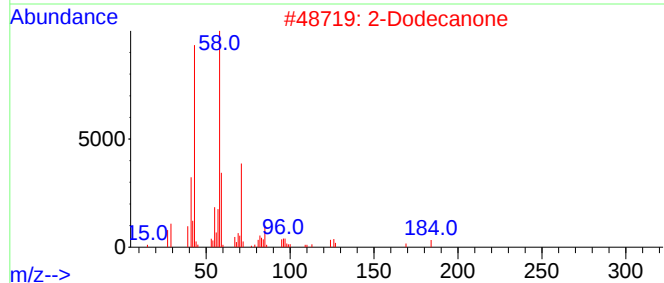
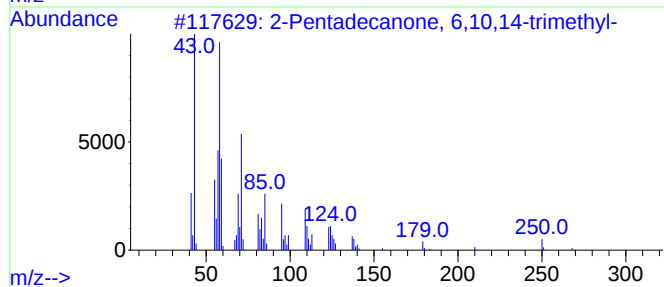
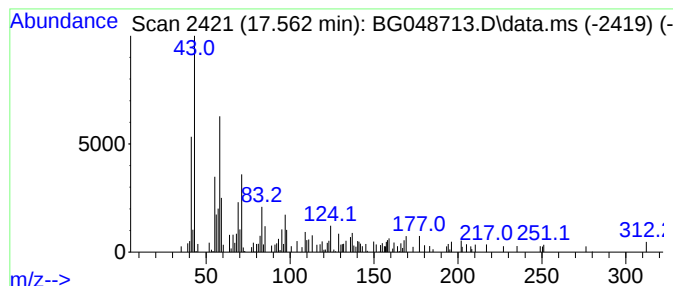
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown17.562 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.562	4.36 ng	77746	Phenanthrene-d10	17.497

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentadecanone, 6,10,14-trimethyl-	268	C18H36O	000502-69-2	47
2		2-Dodecanone	184	C12H24O	006175-49-1	43
3		2-Tridecanone	198	C13H26O	000593-08-8	38
4		2-Decanone	156	C10H20O	000693-54-9	38
5		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
Operator : CG/JU
Sample : M1998-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

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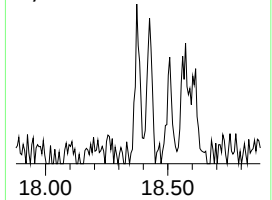
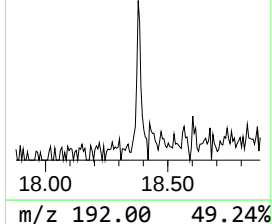
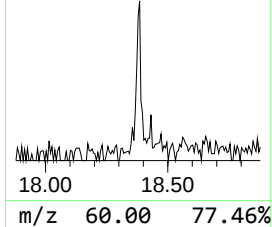
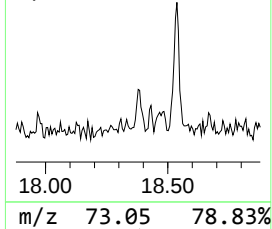
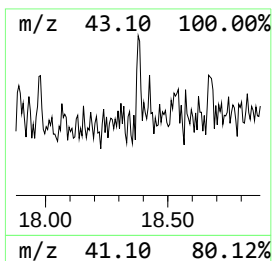
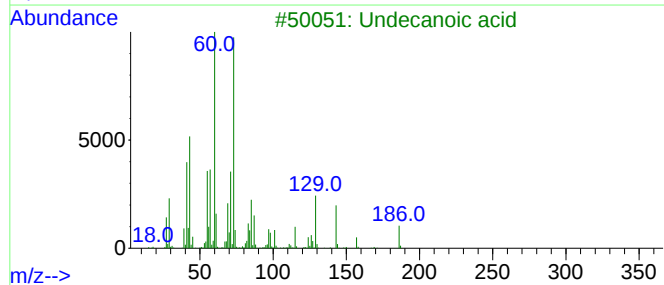
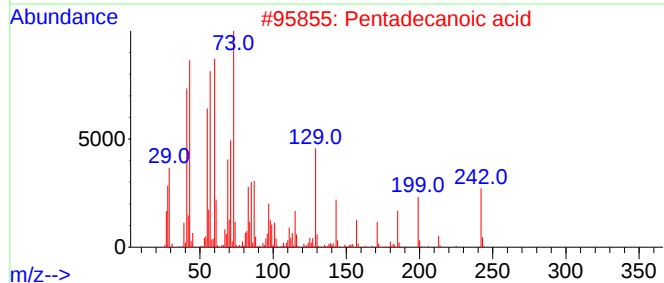
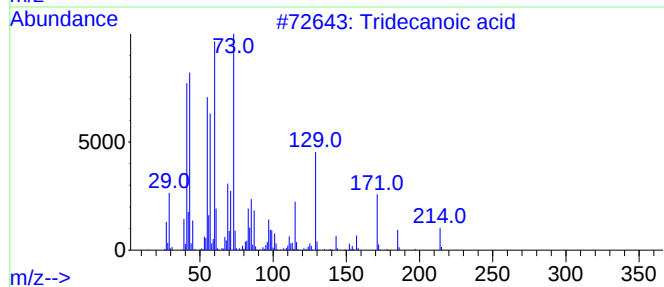
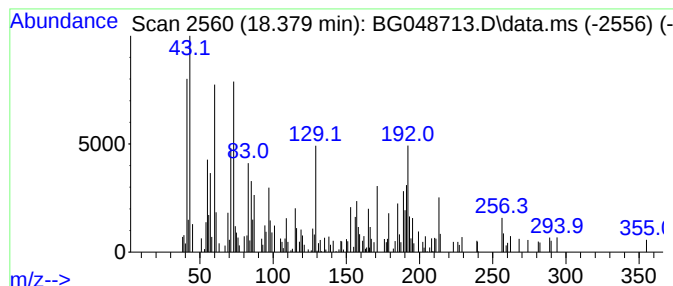
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 unknown18.379 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.379	4.05 ng	72294	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	46
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	35
3			Undecanoic acid	186	C11H22O2	000112-37-8	30
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	30
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
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Sample : M1998-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

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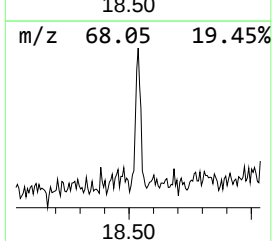
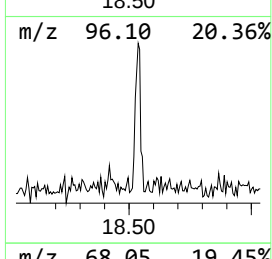
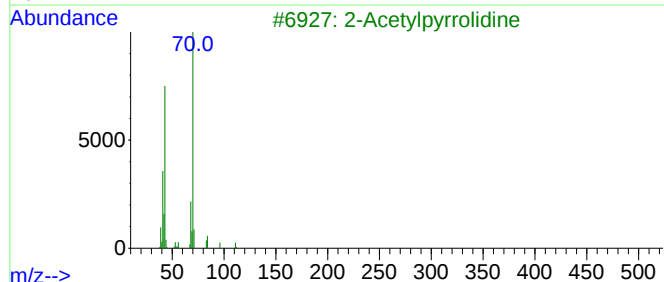
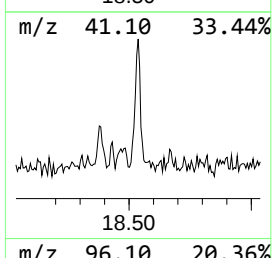
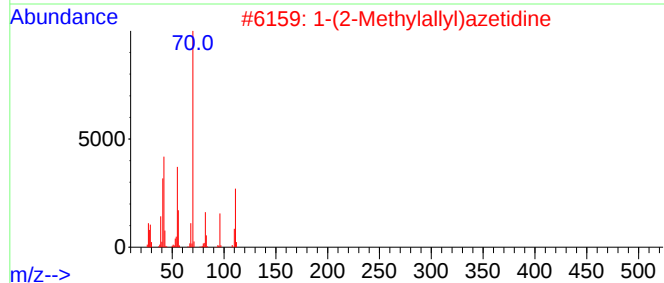
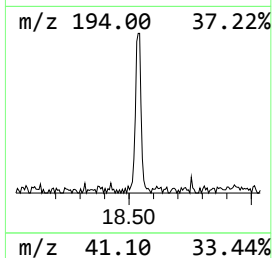
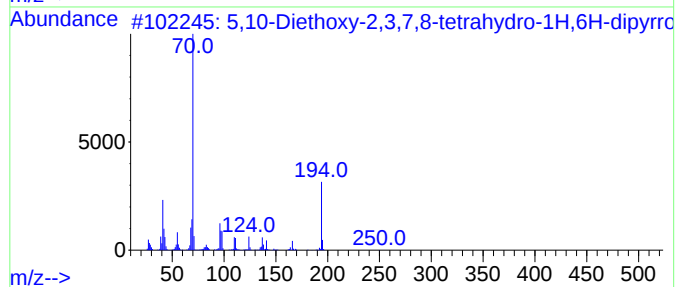
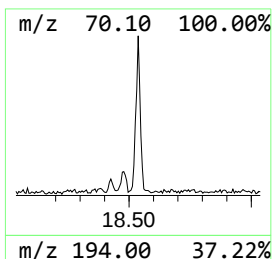
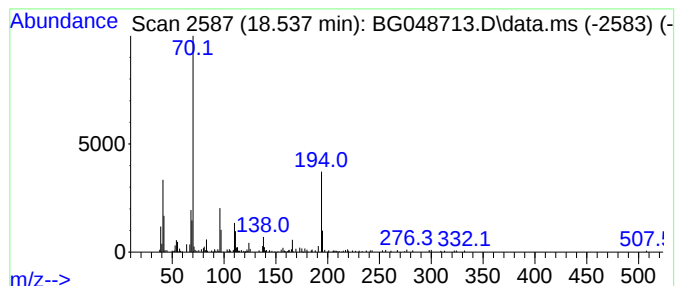
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 5,10-Diethoxy-2,3,7,8-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.537	6.63 ng	118175	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,10-Diethoxy-2,3,7,8-tetrahydro...	250	C14H22N2O2	1000190-75-5	50
2			1-(2-Methylallyl)azetidine	111	C7H13N	1000194-99-1	38
3			2-Acetylpyrrolidine	113	C6H11NO	060026-20-2	37
4			L-Proline, N-(3-cyclopentylpropi...	309	C18H31NO3	1000346-41-0	37
5			L-Proline, N-(3-cyclopentylpropi...	365	C22H39NO3	1000346-41-4	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
Operator : CG/JU
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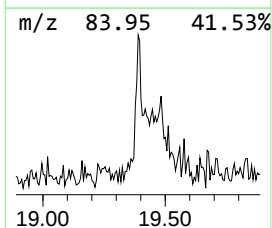
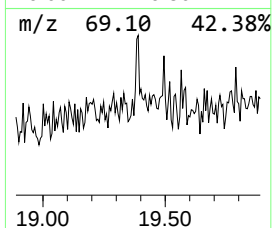
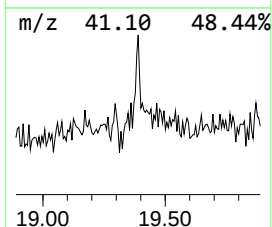
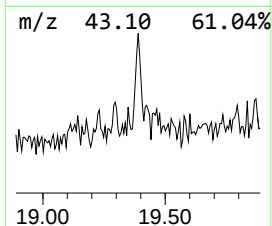
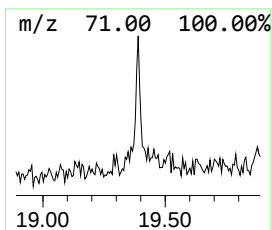
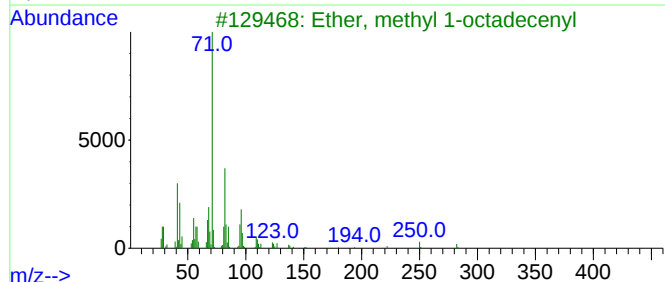
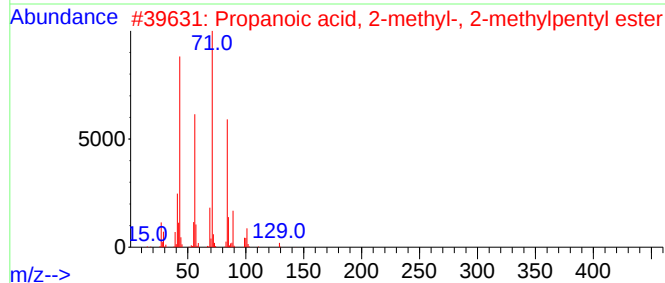
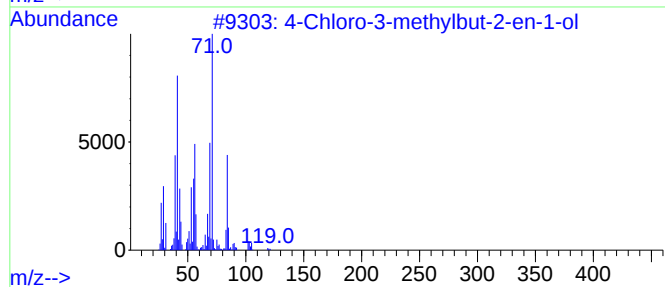
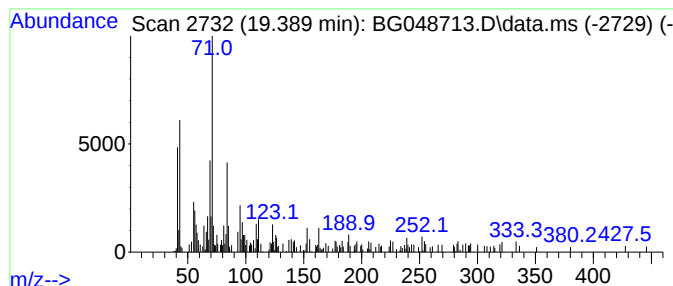
Instrument :
BNA_G
ClientSampleId :
SB-5A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 4-Chloro-3-methylbut-2-en-1-ol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.389	3.21 ng	57231	Phenanthrene-d10		17.497	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4-Chloro-3-methylbut-2-en-1-ol		120	C5H9ClO	053170-97-1	58
2	Propanoic acid, 2-methyl-, 2-met...		172	C10H20O2	084254-82-0	53
3	Ether, methyl 1-octadecenyl		282	C19H38O	026537-06-4	45
4	Cyclopentanol, 1-methyl-		100	C6H12O	001462-03-9	41
5	1,2,4-Oxadiazole-5-carboxamide, ...		333	C16H19N3O5	1000350-15-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
Data File : BG048713.D
Acq On : 15 Apr 2021 17:44
Operator : CG/JU
Sample : M1998-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
SB-5A

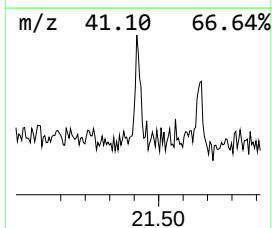
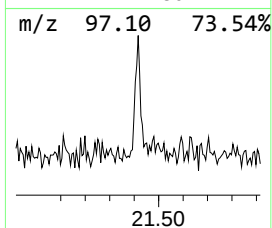
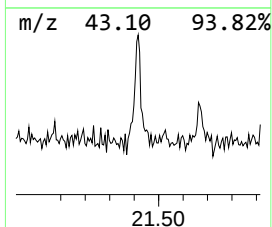
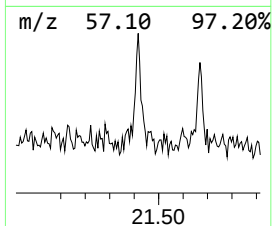
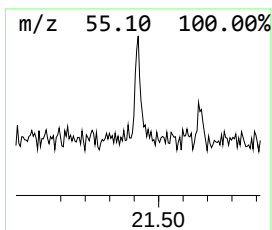
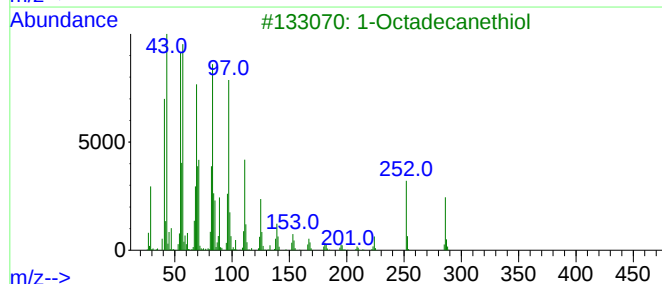
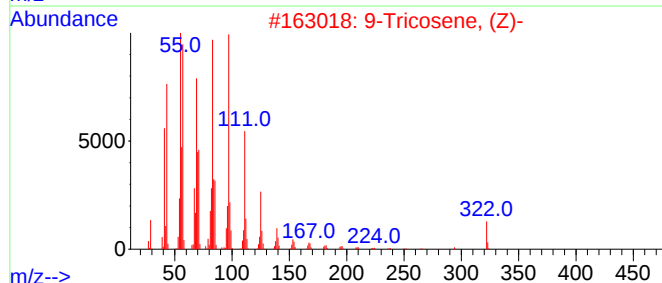
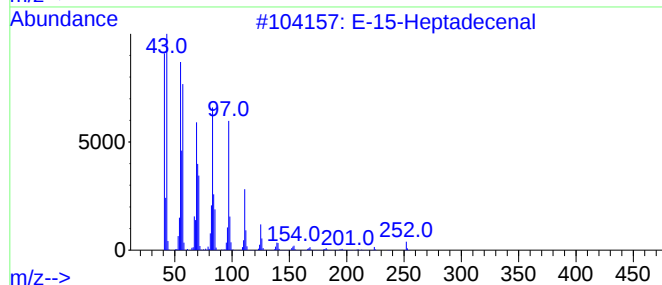
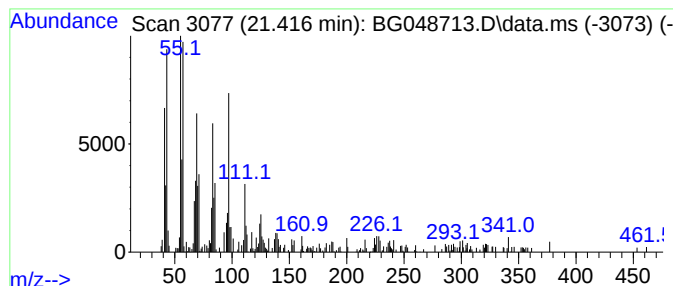
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	7.71 ng	133401	Chrysene-d12	21.798

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2		9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
3		1-Octadecanethiol	286	C18H38S	002885-00-9	93
4		Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	93
5		1-Tricosene	322	C23H46	018835-32-0	92



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041521\
 Data File : BG048713.D
 Acq On : 15 Apr 2021 17:44
 Operator : CG/JU
 Sample : M1998-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-5A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown5.159	5.159	5.3	ng	54237	1	8.085	205856	20.0
1-Hexanol, 2-et...	8.138	11.3	ng	116060	1	8.085	205856	20.0
2-Piperidinone	10.676	56.3	ng	731690	2	10.911	259958	20.0
Indole	12.409	33.8	ng	439291	2	10.911	259958	20.0
unknown12.644	12.644	2.4	ng	30785	2	10.911	259958	20.0
unknown13.549	13.549	2.4	ng	42080	3	14.742	346001	20.0
unknown14.577	14.577	2.3	ng	39445	3	14.742	346001	20.0
unknown15.224	15.224	2.4	ng	41123	3	14.742	346001	20.0
unknown15.529	15.529	2.3	ng	39121	3	14.742	346001	20.0
Hexadecane	16.457	6.3	ng	112808	4	17.497	356600	20.0
1-Adamantyl m-t...	16.563	2.1	ng	37633	4	17.497	356600	20.0
unknown16.880	16.880	2.0	ng	36322	4	17.497	356600	20.0
unknown17.010	17.010	4.2	ng	74025	4	17.497	356600	20.0
unknown17.250	17.250	12.8	ng	228536	4	17.497	356600	20.0
unknown17.562	17.562	4.4	ng	77746	4	17.497	356600	20.0
unknown18.379	18.379	4.0	ng	72294	4	17.497	356600	20.0
5,10-Diethoxy-2...	18.537	6.6	ng	118175	4	17.497	356600	20.0
4-Chloro-3-meth...	19.389	3.2	ng	57231	4	17.497	356600	20.0
E-15-Heptadecenal	21.416	7.7	ng	133401	5	21.798	345945	20.0