

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
 Data File : BG056443.D
 Acq On : 26 Jan 2023 15:05
 Operator : CG/JU
 Sample : 01289-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VNJ209-STOCK

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-BG122722.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056443.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.333	341	348	355	rBB	88303	140005	6.29%	1.216%
2	5.815	423	430	443	rVB	380415	607946	27.32%	5.281%
3	7.436	699	706	718	rBV	387577	663362	29.81%	5.762%
4	8.294	844	852	859	rBB	94650	162870	7.32%	1.415%
5	9.469	1044	1052	1062	rVB	222473	395316	17.76%	3.434%
6	11.126	1327	1334	1344	rBB	130359	236935	10.65%	2.058%
7	13.423	1717	1725	1729	rBV6	9980	24265	1.09%	0.211%
8	13.535	1737	1744	1753	rBV	860710	1302624	58.53%	11.314%
9	13.940	1806	1813	1820	rVB5	35811	77437	3.48%	0.673%
10	14.833	1960	1965	1969	rBV2	34764	48424	2.18%	0.421%
11	14.910	1971	1978	1987	rVV	270593	430072	19.32%	3.736%
12	15.104	2005	2011	2014	rBV7	13064	26185	1.18%	0.227%
13	15.697	2108	2112	2118	rBV6	13761	29322	1.32%	0.255%
14	15.809	2123	2131	2137	rVV	55628	102685	4.61%	0.892%
15	15.914	2145	2149	2151	rBV3	18085	25169	1.13%	0.219%
16	16.126	2181	2185	2189	rVB4	21810	31915	1.43%	0.277%
17	16.249	2201	2206	2217	rVB	167972	289807	13.02%	2.517%
18	16.390	2224	2230	2235	rBV	648514	983208	44.18%	8.540%
19	16.860	2306	2310	2318	rVB4	33730	59897	2.69%	0.520%
20	17.007	2331	2335	2342	rVB	131209	177213	7.96%	1.539%
21	17.078	2343	2347	2351	rVB	50000	66161	2.97%	0.575%
22	17.648	2438	2444	2448	rBV	355585	524871	23.58%	4.559%
23	17.689	2448	2451	2458	rVB	81901	113097	5.08%	0.982%
24	17.759	2459	2463	2468	rBV2	45355	61482	2.76%	0.534%
25	17.912	2486	2489	2492	rBV3	42937	48559	2.18%	0.422%
26	18.400	2568	2572	2578	rVB	72836	118339	5.32%	1.028%
27	18.553	2595	2598	2603	rVB3	59689	70106	3.15%	0.609%
28	18.670	2615	2618	2620	rBV2	27616	35569	1.60%	0.309%
29	18.970	2664	2669	2673	rBV	144097	220839	9.92%	1.918%
30	19.005	2673	2675	2681	rVB	63891	82945	3.73%	0.720%
31	19.340	2729	2732	2737	rVB2	110900	126576	5.69%	1.099%
32	19.598	2774	2776	2779	rVB	35414	30887	1.39%	0.268%
33	19.880	2821	2824	2830	rVB2	87054	110021	4.94%	0.956%
34	19.945	2833	2835	2837	rBV2	28806	28579	1.28%	0.248%
35	20.045	2848	2852	2855	rVB	63162	68615	3.08%	0.596%
36	20.221	2877	2882	2888	rBV	1738493	2225602	100.00%	19.331%

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

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

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
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37	20.403	2911	2913	2918	rVB	47611	50412	2.27%	0.438%
38	21.155	3038	3041	3045	rVB	67399	74885	3.36%	0.650%
39	21.514	3099	3102	3110	rVB4	60125	101765	4.57%	0.884%
40	21.678	3126	3130	3136	rVB2	49283	76879	3.45%	0.668%
41	21.837	3155	3157	3165	rVB4	36478	58811	2.64%	0.511%
42	21.937	3168	3174	3182	rVB2	382416	650980	29.25%	5.654%
43	23.247	3393	3397	3402	rVB3	32436	60998	2.74%	0.530%
44	25.368	3749	3758	3772	rVB	233203	691281	31.06%	6.004%

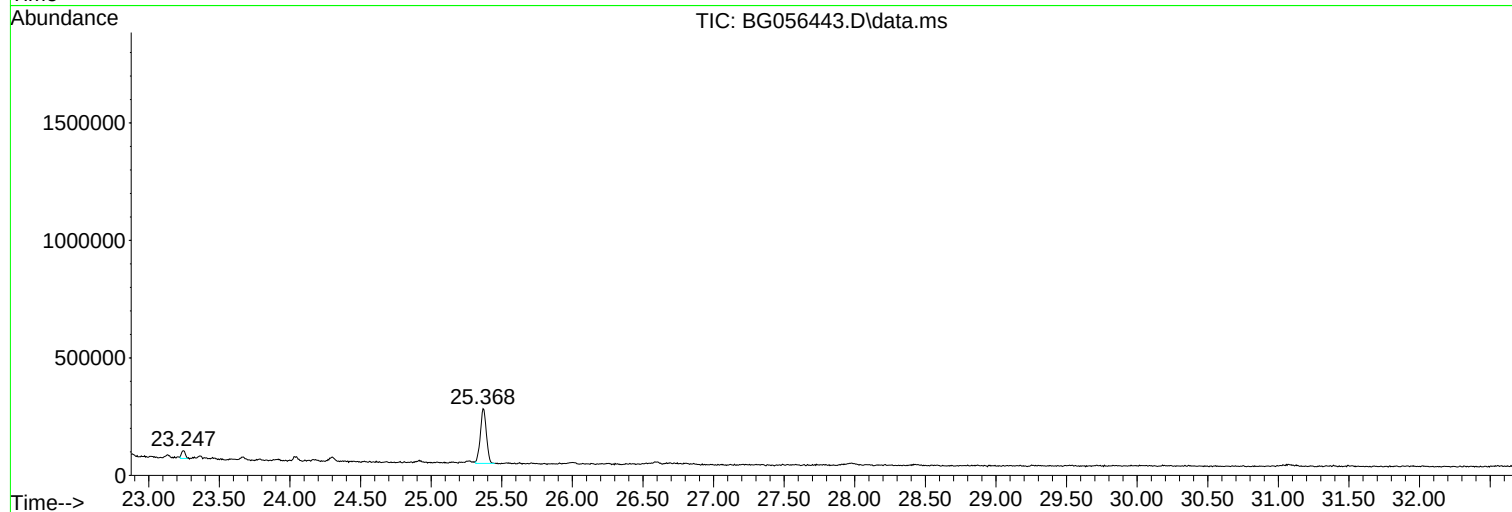
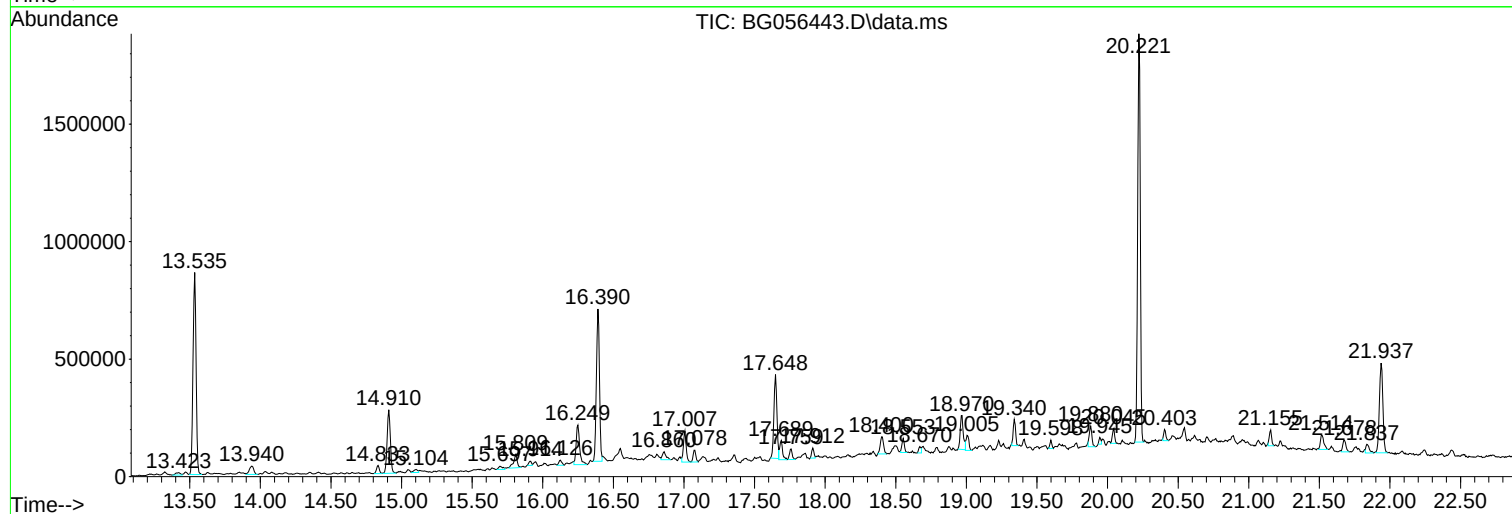
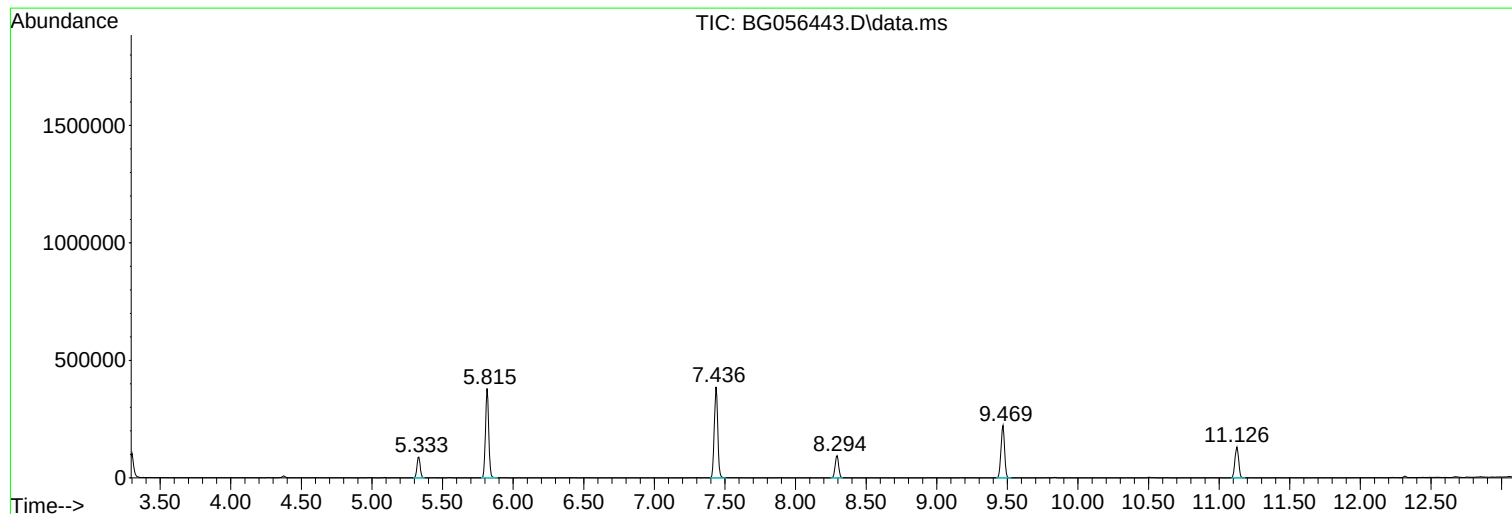
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : 01289-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

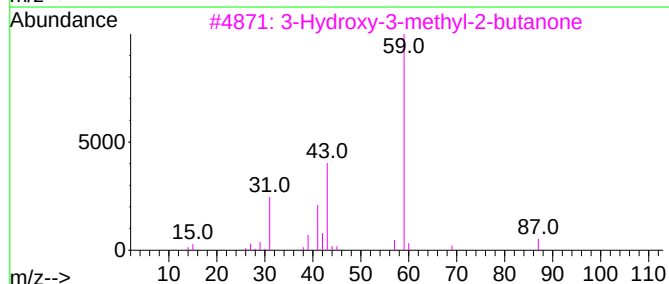
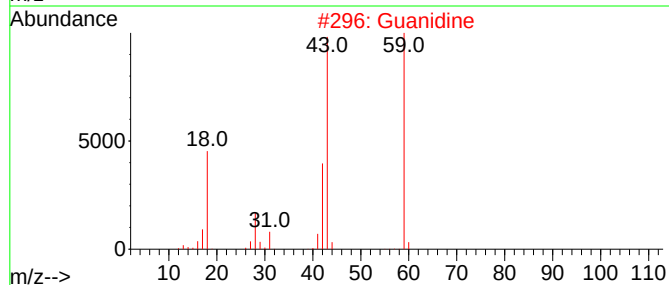
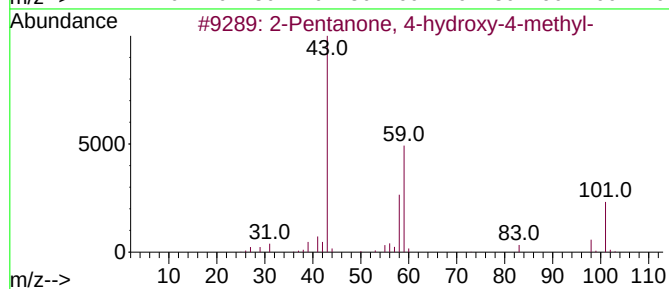
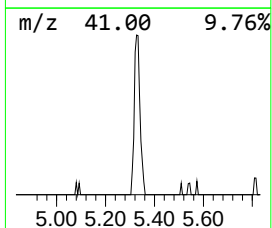
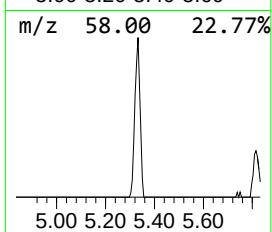
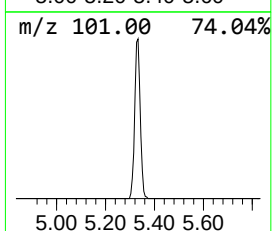
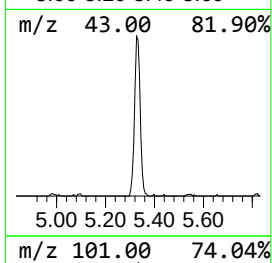
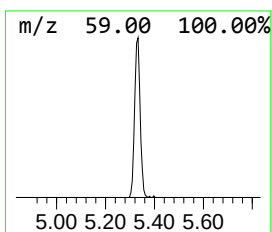
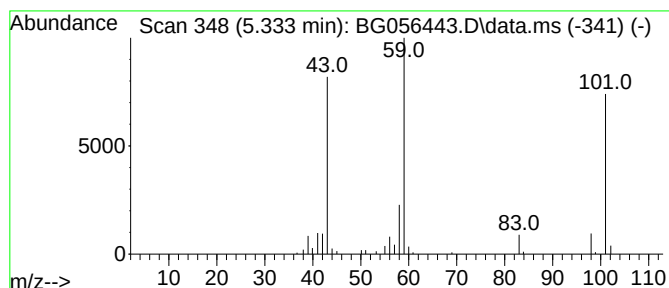
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.333	17.19 ng	140005	1,4-Dichlorobenzene-d4	8.294	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	43
2	Guanidine	59	CH5N3	000113-00-8	25
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	10
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	10



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Misc :
ALS Vial : 9 Sample Multiplier: 1

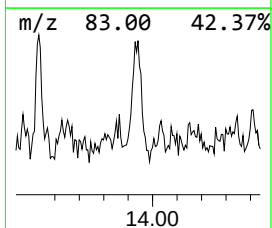
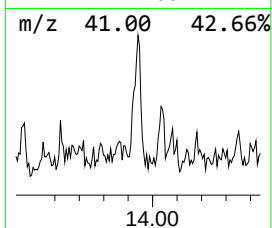
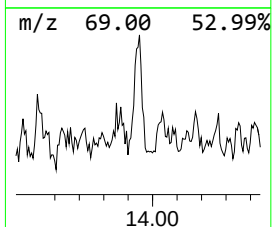
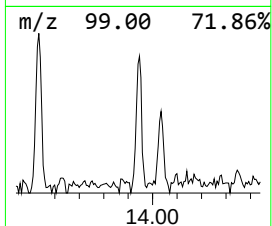
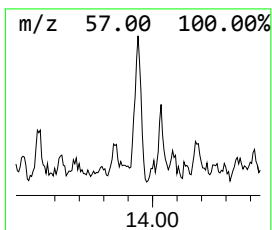
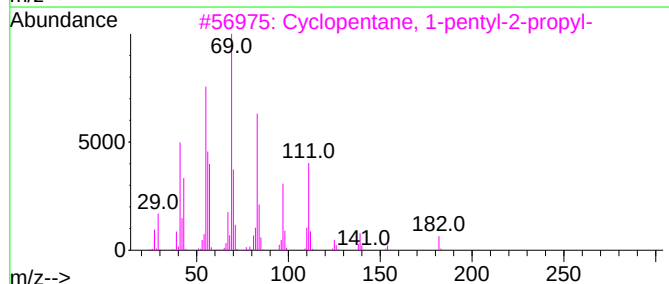
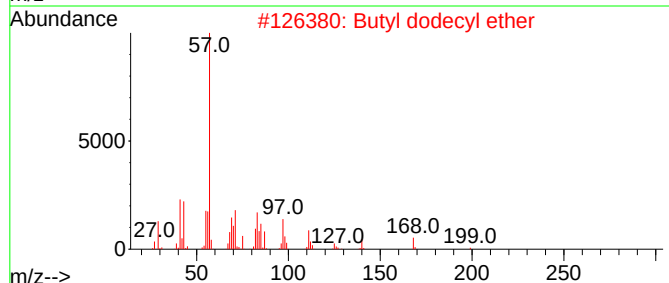
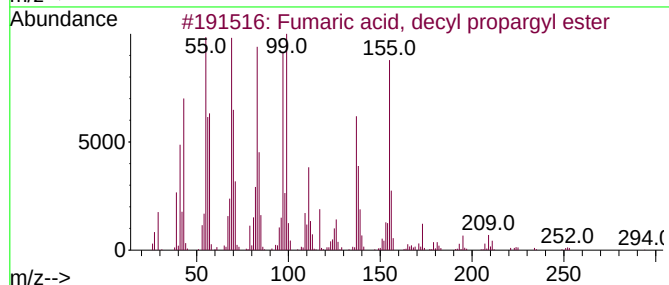
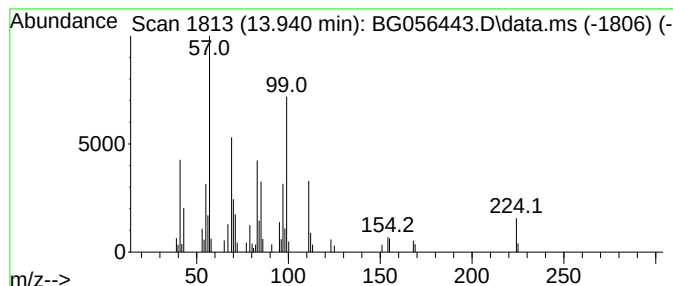
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Fumaric acid, decyl proparg... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.940	3.60 ng	77437	Acenaphthene-d10		14.910	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Fumaric acid, decyl propargyl ester		294	C17H26O4	1000330-53-4	50
2	Butyl dodecyl ether		242	C16H34O	1000406-40-3	50
3	Cyclopentane, 1-pentyl-2-propyl-		182	C13H26	062199-51-3	47
4	Sulfurous acid, butyl tetradecyl...		334	C18H38O3S	1010309-18-1	43
5	1-Hexadecanol		242	C16H34O	036653-82-4	43



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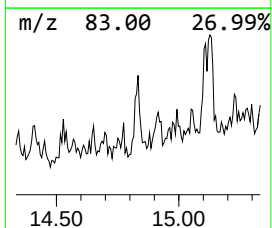
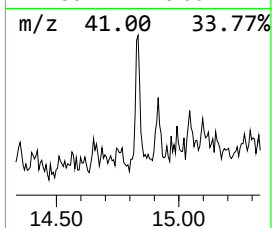
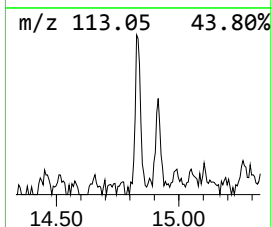
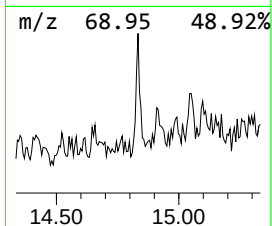
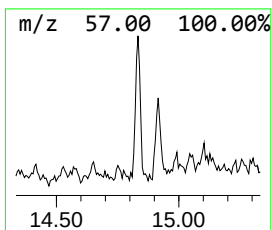
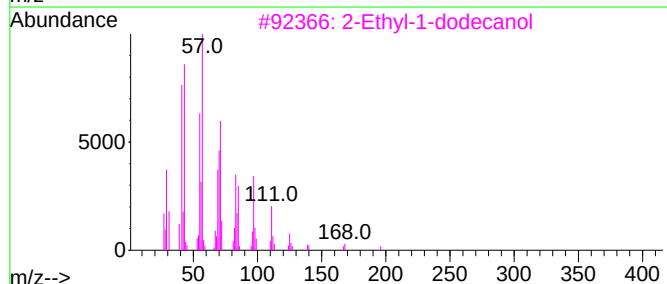
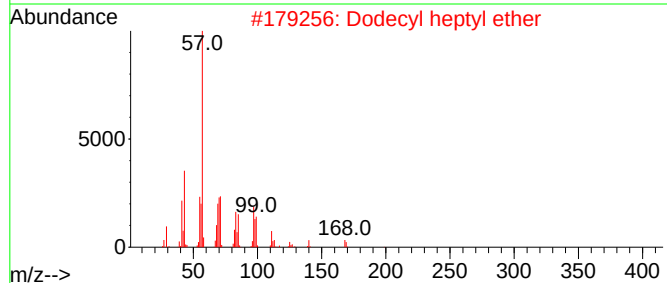
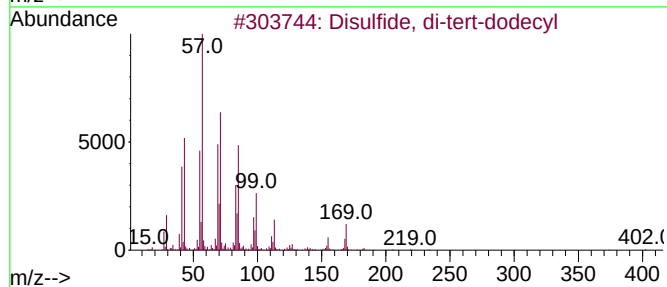
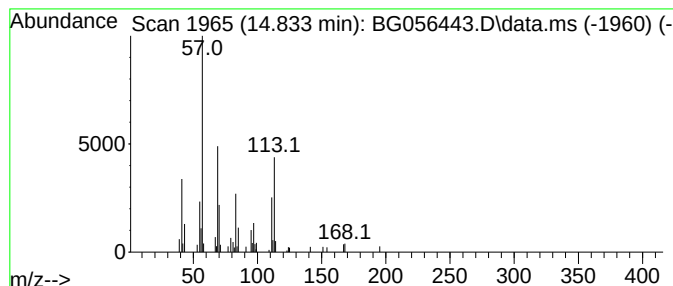
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown14.833 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	2.25 ng	48424	Acenaphthene-d10	14.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	37
2			Dodecyl heptyl ether	284	C19H40O	1010406-39-2	32
3			2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	32
4			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	25
5			Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	25



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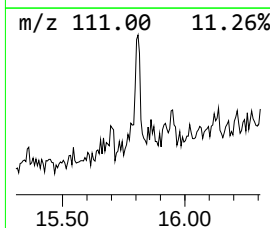
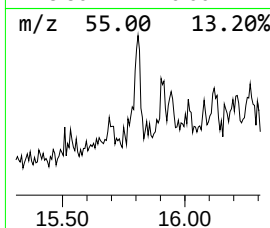
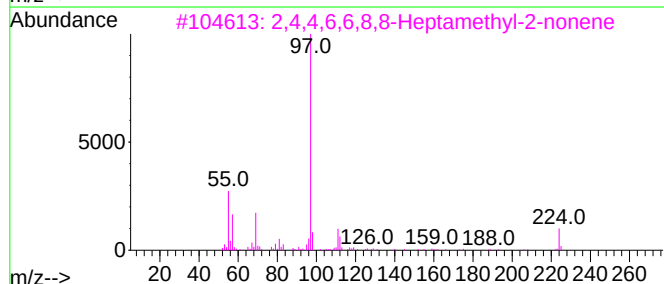
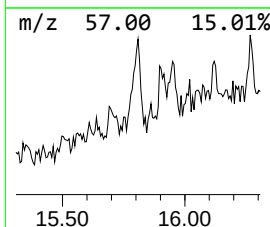
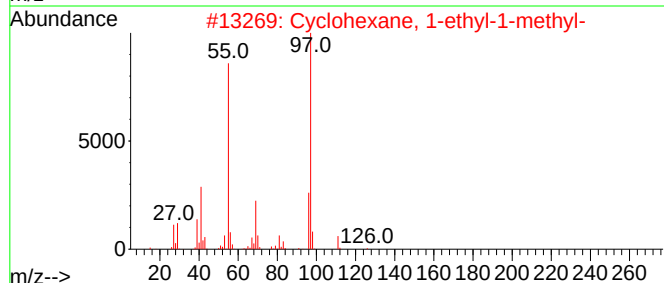
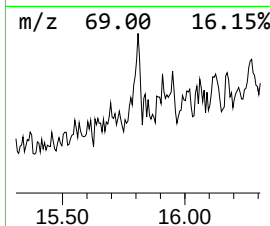
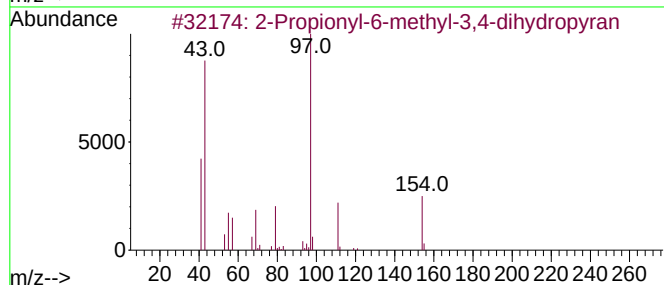
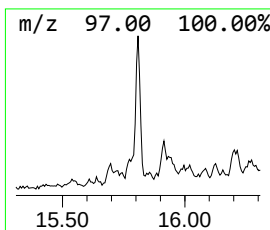
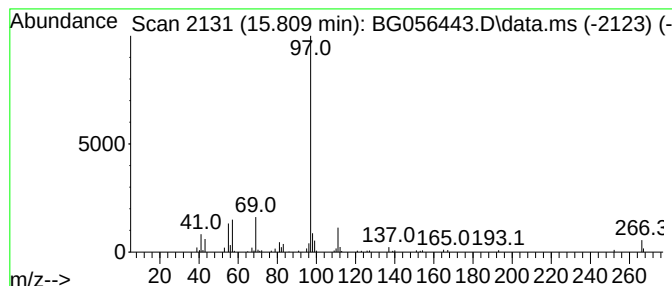
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Propionyl-6-methyl-3,4-di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.809	4.78 ng	102685	Acenaphthene-d10	14.910

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propionyl-6-methyl-3,4-dihydro...	154	C9H14O2	1000145-07-7	64
2		Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	59
3		2,4,4,6,6,8,8-Heptamethyl-2-nonene	224	C16H32	039761-73-4	56
4		Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	50
5		Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1010309-22-7	50



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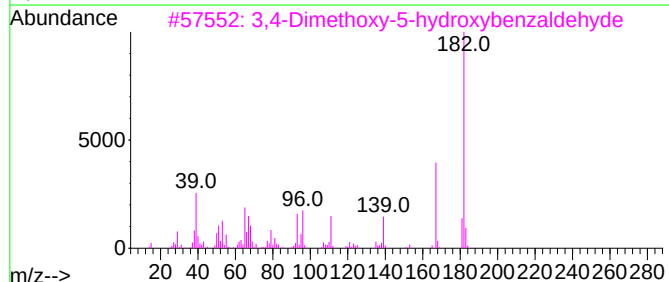
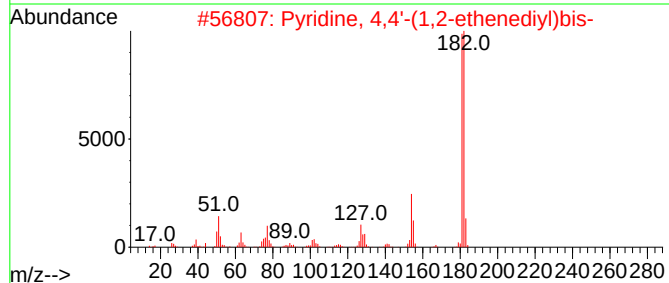
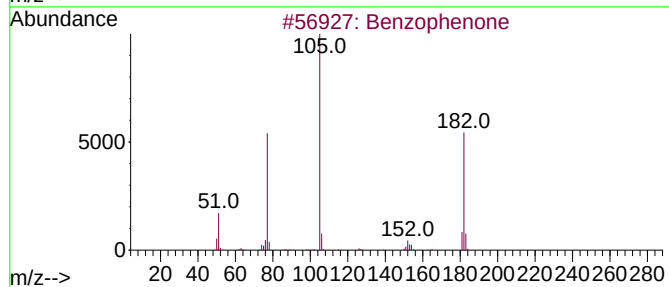
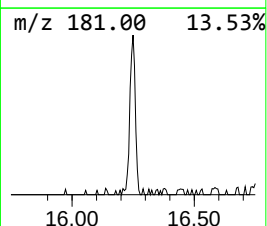
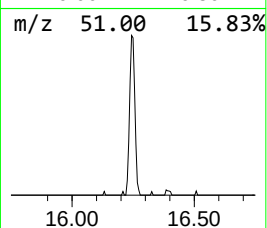
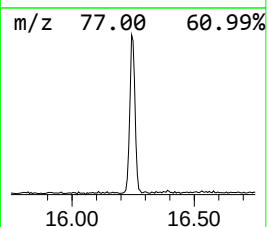
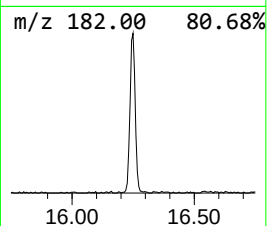
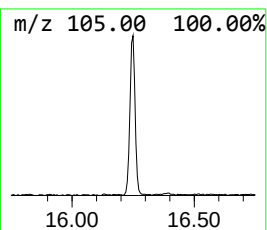
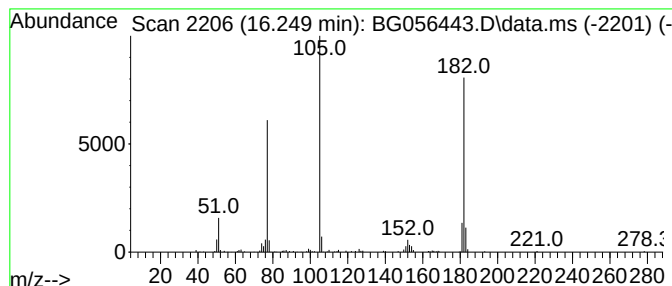
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.249	13.48 ng	289807	Acenaphthene-d10	14.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Pyridine, 4,4'-(1,2-ethenediyl)bis-	182	C12H10N2	001135-32-6	47
3			3,4-Dimethoxy-5-hydroxybenzaldehyde	182	C9H10O4	029865-90-5	47
4			Azobenzene	182	C12H10N2	000103-33-3	43
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
Acq On : 26 Jan 2023 15:05
Operator : CG/JU
Sample : 01289-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ209-STOCK

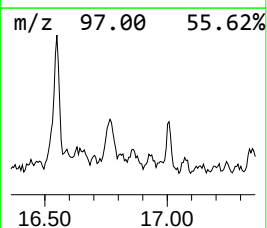
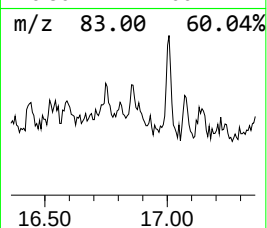
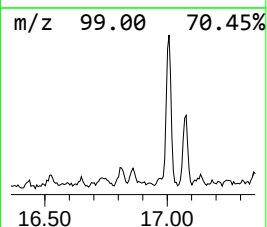
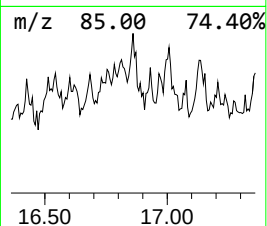
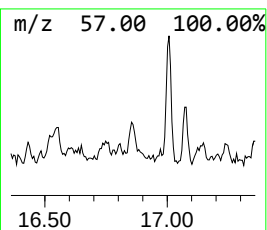
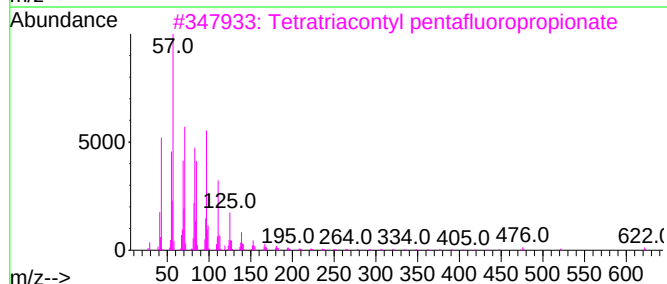
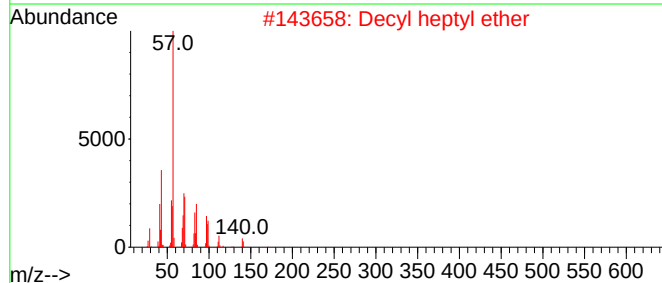
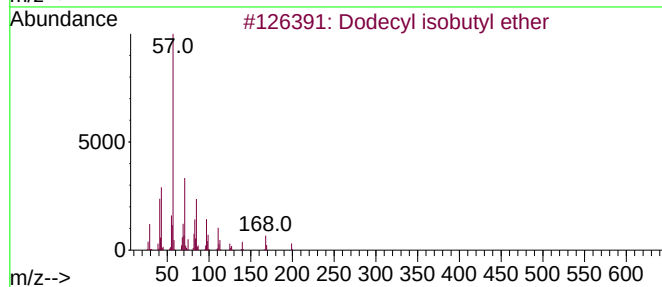
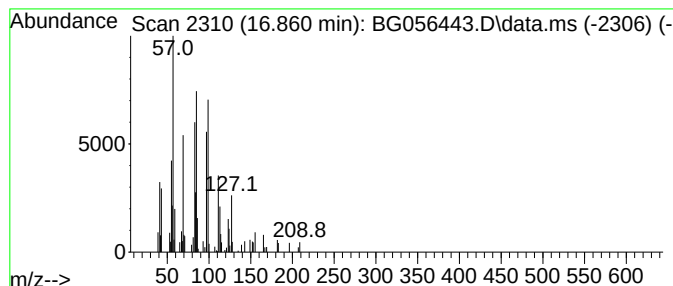
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dodecyl isobutyl ether Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.860	2.28 ng	59897	Phenanthrene-d10	17.648

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecyl isobutyl ether	242	C16H34O	1000406-32-6	53
2			Decyl heptyl ether	256	C17H36O	1000406-39-1	50
3			Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	37
4			Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	32
5			2-Propanone, 1,1,3,3-tetrachloro-	194	C3H2Cl4O	000632-21-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
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Acq On : 26 Jan 2023 15:05
Operator : CG/JU
Sample : 01289-01
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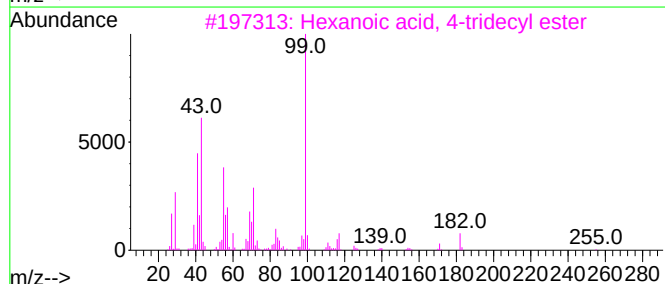
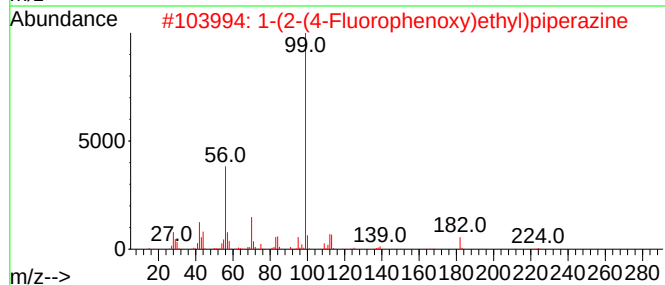
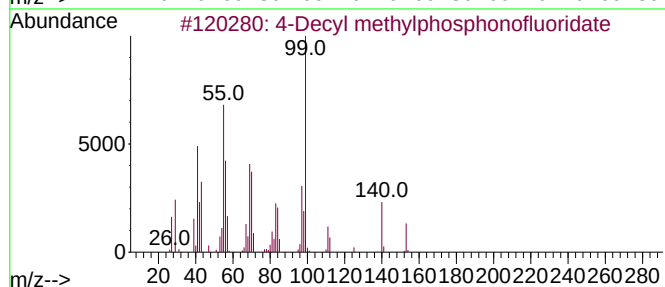
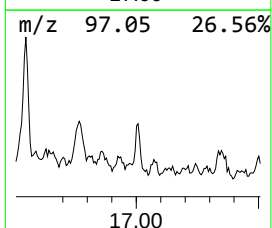
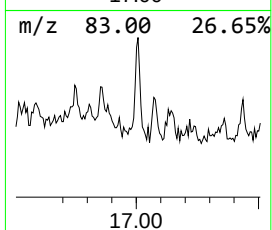
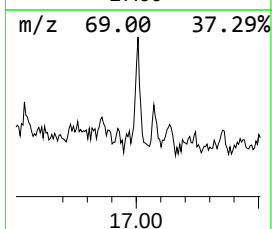
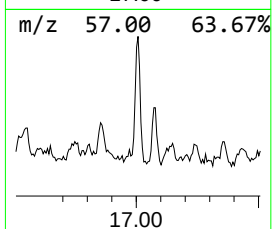
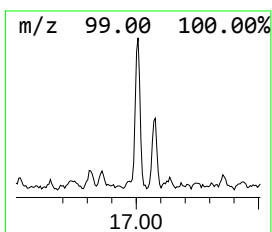
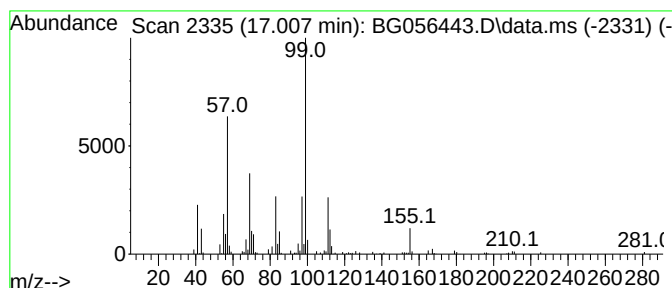
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4-Decyl methylphosphonofluo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.007	6.75 ng	177213	Phenanthrene-d10	17.648

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Decyl methylphosphonofluoridate	238	C11H24F02P	1000216-71-5	64
2			1-(2-(4-Fluorophenoxy)ethyl)pipe...	224	C12H17FN2O	077602-92-7	43
3			Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	43
4			Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	43
5			1,1'-Ethane-1,2-diylpiperazine	198	C10H22N4	019479-83-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
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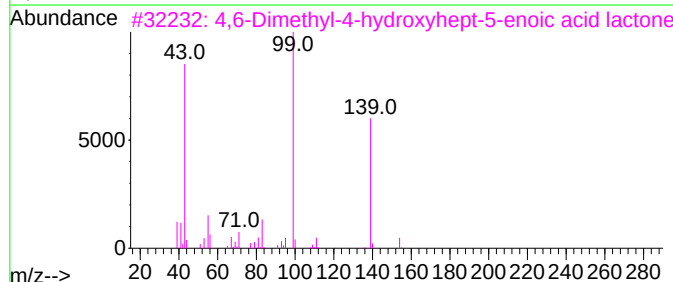
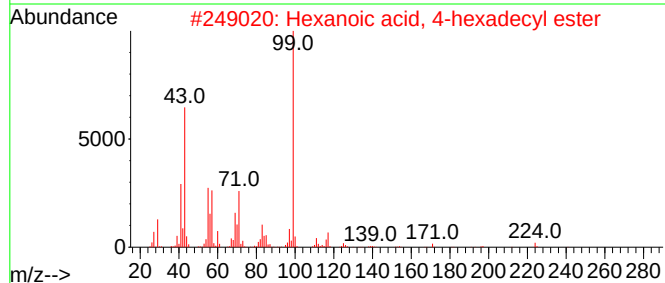
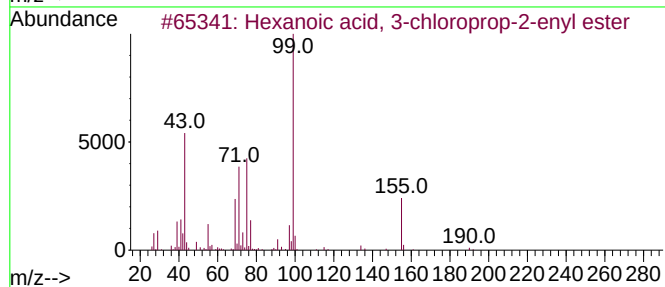
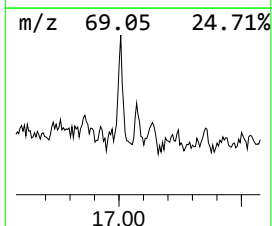
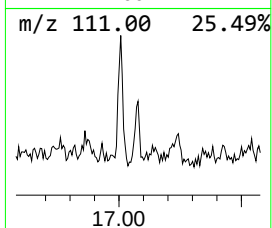
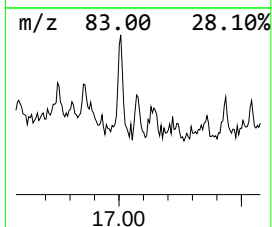
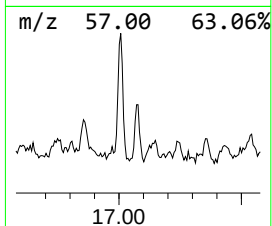
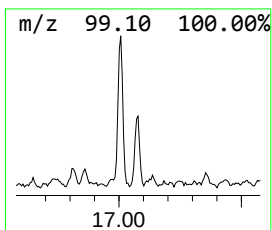
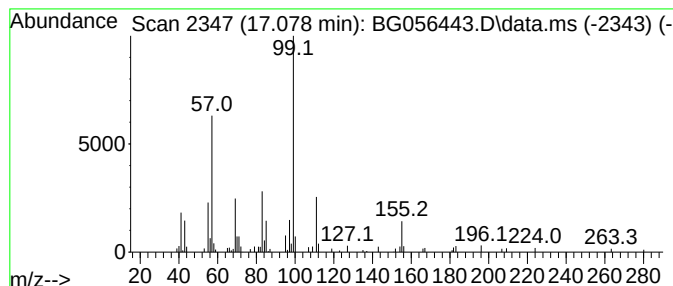
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.078 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.078	2.52 ng	66161	Phenanthrene-d10	17.648	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	47
2	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	40
3	4,6-Dimethyl-4-hydroxyhept-5-eno...	154	C9H14O2	1000122-47-0	38
4	2-Butenedioic acid (Z)-, dibutyl...	228	C12H20O4	000105-76-0	37
5	Pyrrol-2(5H)-one, 4-acetyl-5-(2-...	363	C18H22ClN3O3	302566-40-1	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
Acq On : 26 Jan 2023 15:05
Operator : CG/JU
Sample : 01289-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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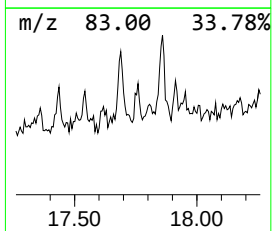
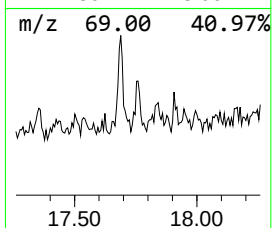
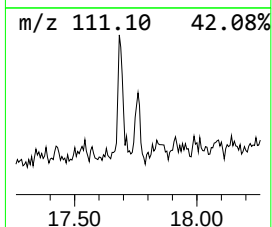
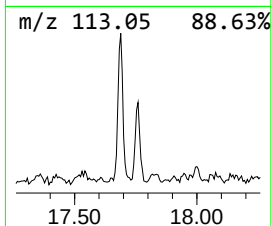
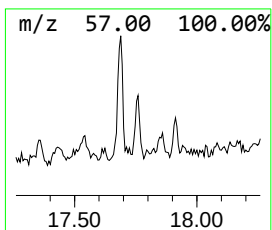
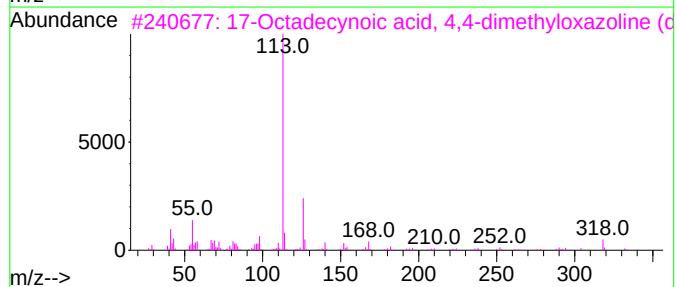
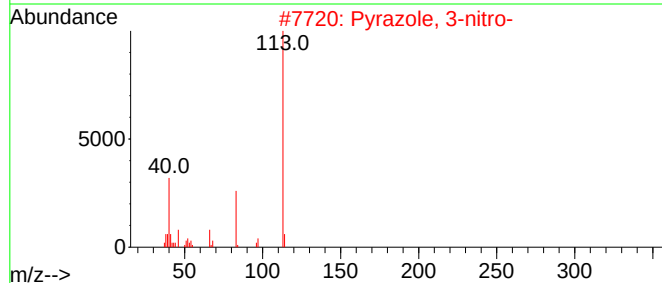
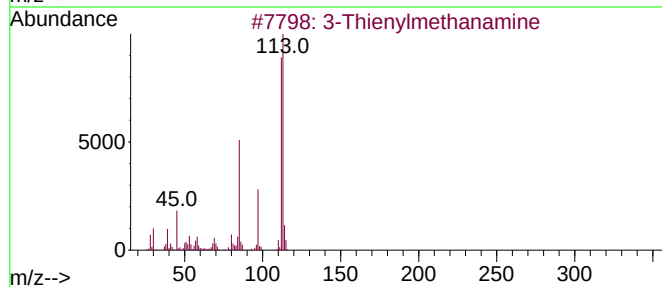
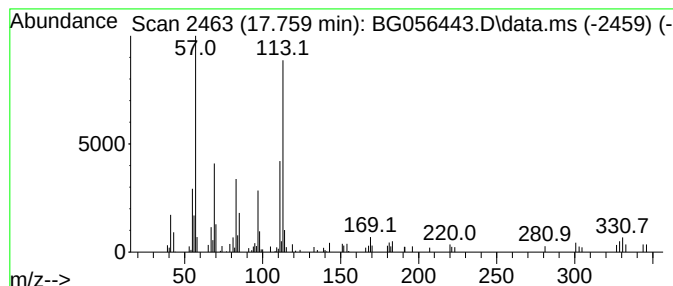
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.759 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.759	2.34 ng	61482	Phenanthrene-d10	17.648

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Thienylmethanamine	113	C5H7NS	027757-86-4	47
2			Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	43
3			17-Octadecynoic acid, 4,4-dimeth...	333	C22H39NO	1000333-54-1	38
4			Pyrrolidine, 1-(1-oxooctadecyl)-	337	C22H43NO	033707-76-5	38
5			Pyrrolidine, 1-(1-oxo-17-octadec...	335	C22H41NO	052380-50-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
Acq On : 26 Jan 2023 15:05
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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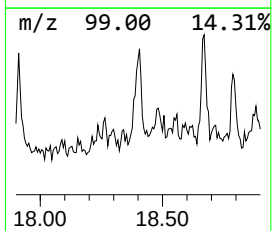
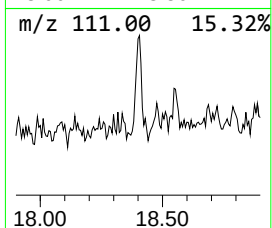
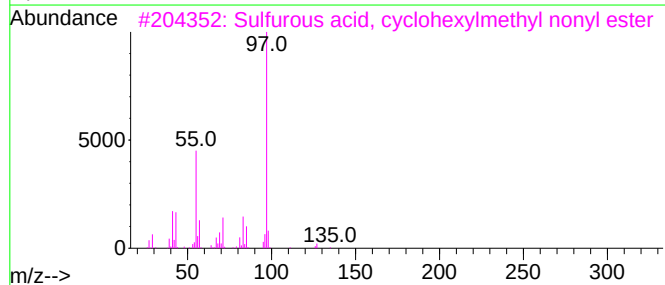
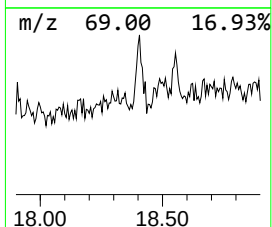
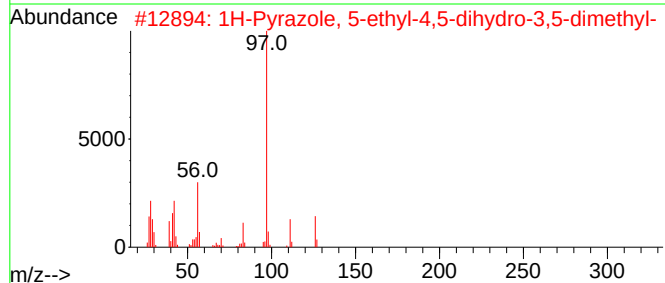
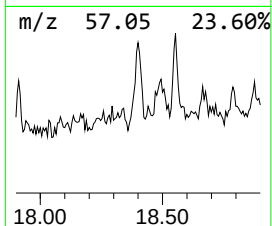
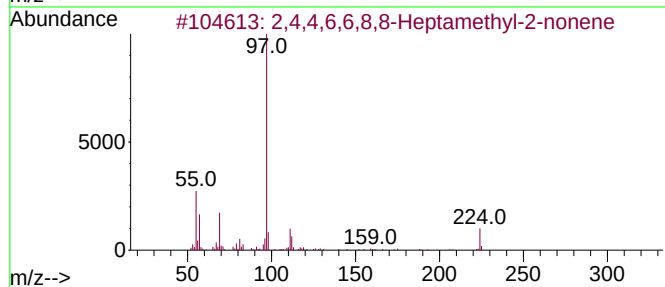
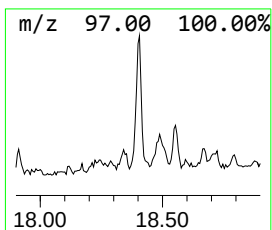
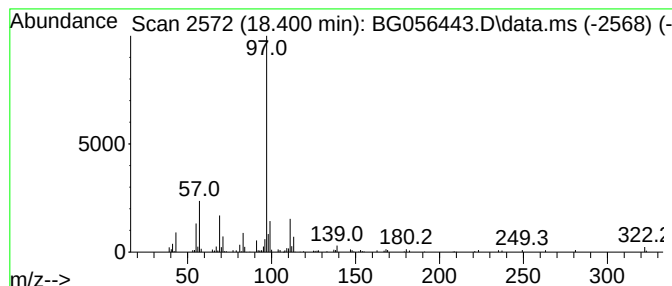
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2,4,4,6,6,8,8-Heptamethyl-2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.400	4.51 ng	118339	Phenanthrene-d10	17.648

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	56	
2	1H-Pyrazole, 5-ethyl-4,5-dihydro...	126	C7H14N2	021981-22-6	53	
3	Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	53	
4	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	53	
5	Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1010309-22-7	53	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
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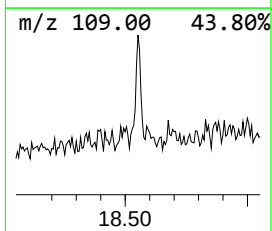
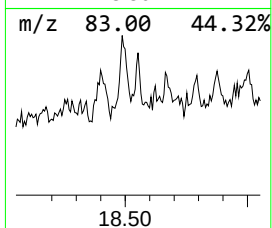
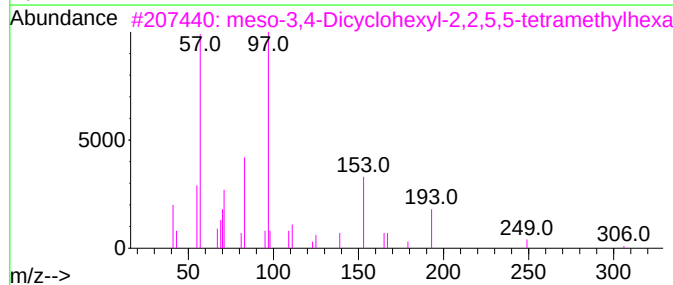
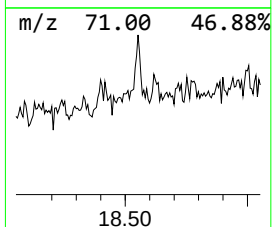
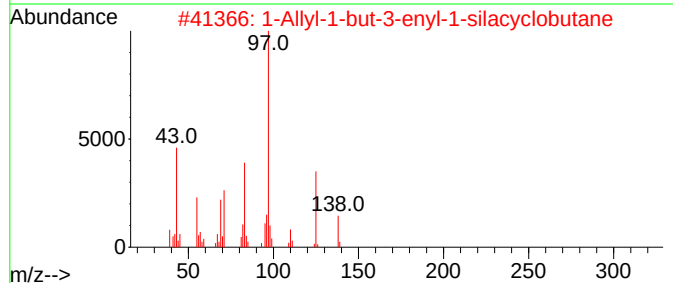
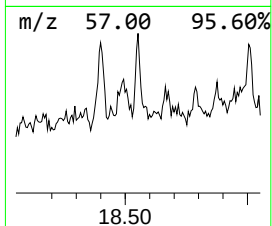
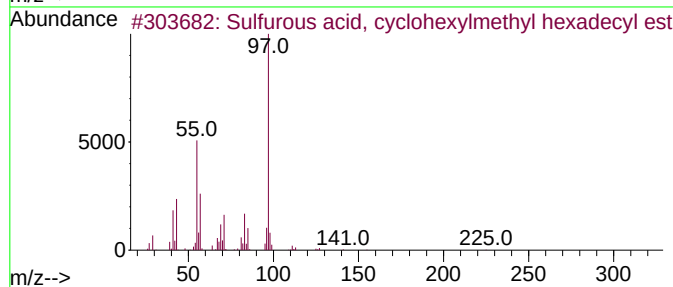
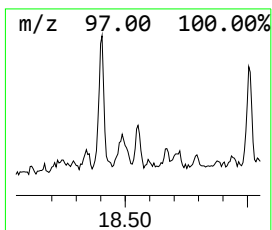
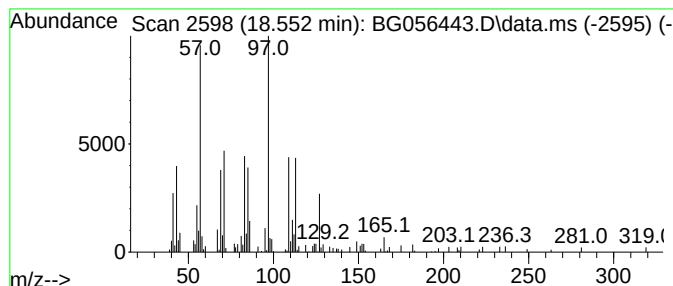
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown18.552 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.552	2.67 ng	70106	Phenanthrene-d10	17.648

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	37
2			1-Allyl-1-but-3-enyl-1-silacyclo...	166	C10H18Si	127597-51-7	35
3			meso-3,4-Dicyclohexyl-2,2,5,5-te...	306	C22H42	065149-86-2	32
4			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	22
5			3,3,7,7-Tetramethyl-5-oxa-1,9-di...	182	C10H18N2O	090832-25-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
Acq On : 26 Jan 2023 15:05
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ALS Vial : 9 Sample Multiplier: 1

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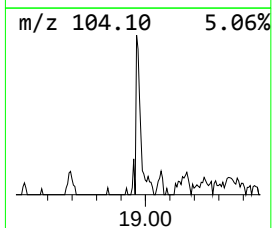
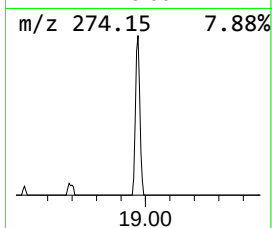
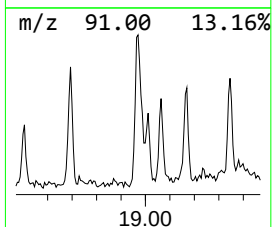
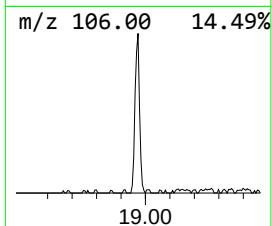
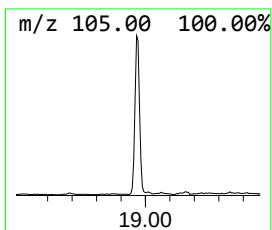
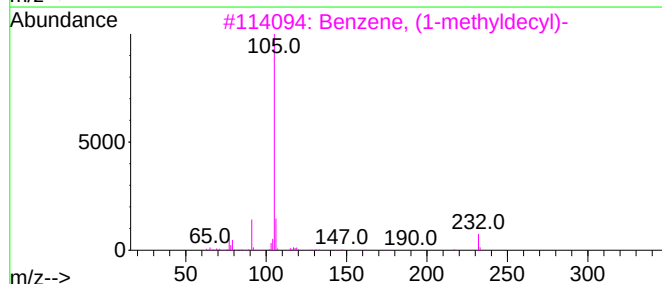
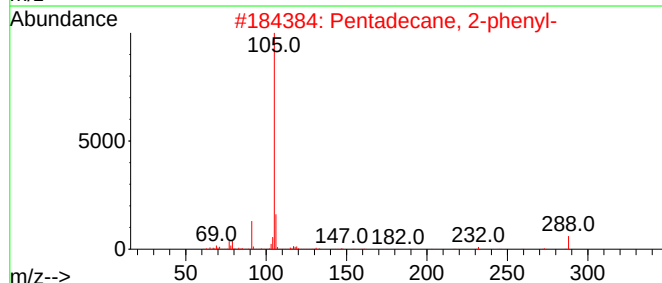
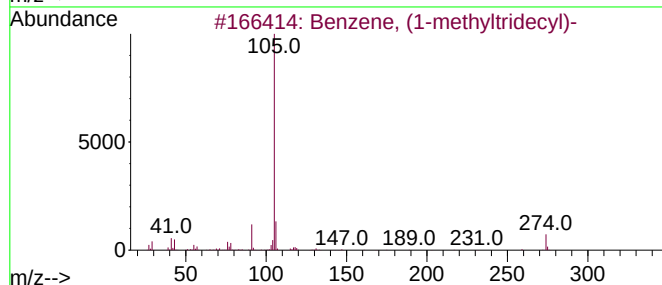
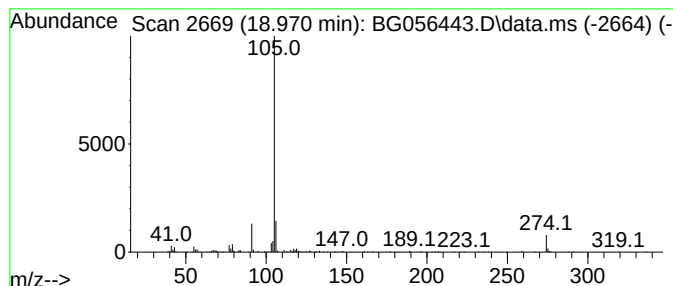
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzene, (1-methyltridecyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.970	8.41 ng	220839	Phenanthrene-d10	17.648

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	87
2		Pentadecane, 2-phenyl-	288	C21H36	004534-66-1	68
3		Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	64
4		Benzene, (1-methylheptyl)-	190	C14H22	000777-22-0	59
5		Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
Acq On : 26 Jan 2023 15:05
Operator : CG/JU
Sample : 01289-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

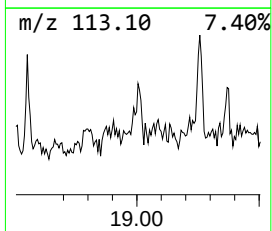
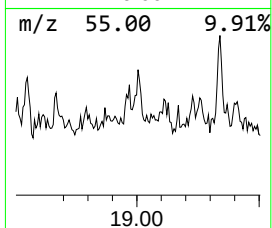
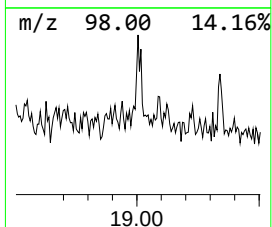
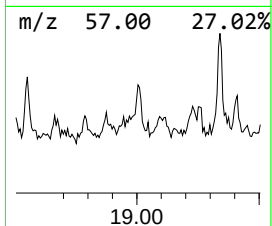
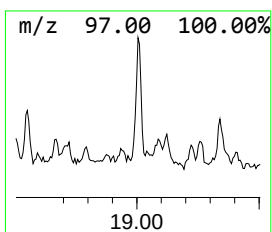
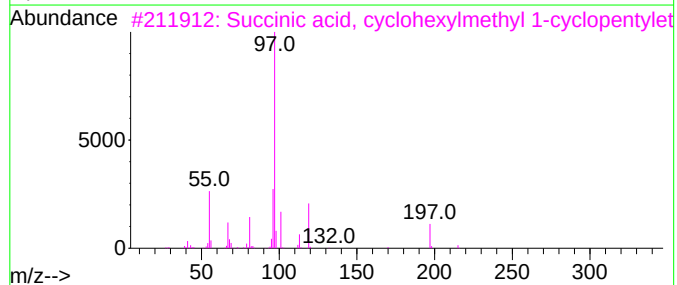
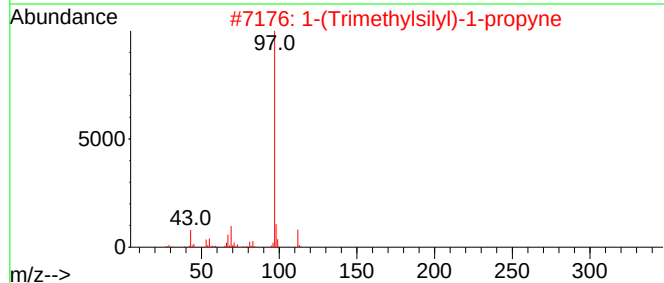
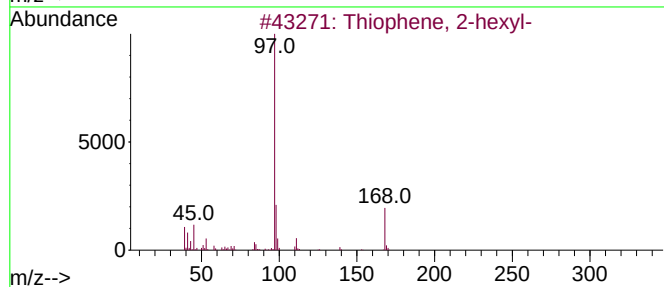
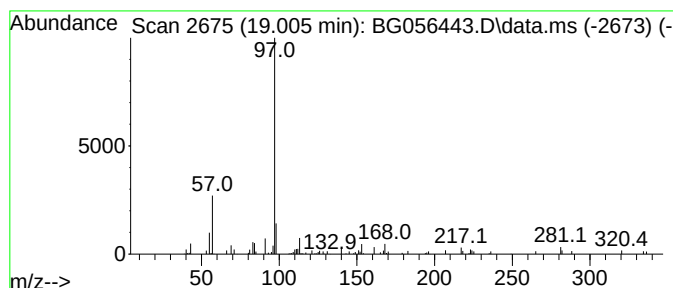
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Thiophene, 2-hexyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.005	3.16 ng	82945	Phenanthrene-d10	17.648
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		Thiophene, 2-hexyl-	168 C10H16S	018794-77-9 64
2		1-(Trimethylsilyl)-1-propyne	112 C6H12Si	006224-91-5 50
3		Succinic acid, cyclohexylmethyl ...	310 C18H30O4	1000391-41-3 50
4		Cyclohexane, 1,3-dimethyl-, cis-	112 C8H16	000638-04-0 50
5		Bis(2-isopropyl-5-methylcyclohex...	372 C21H41O3P	1000510-36-7 45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
Acq On : 26 Jan 2023 15:05
Operator : CG/JU
Sample : 01289-01
Misc :
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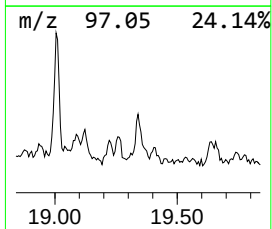
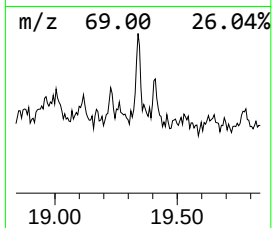
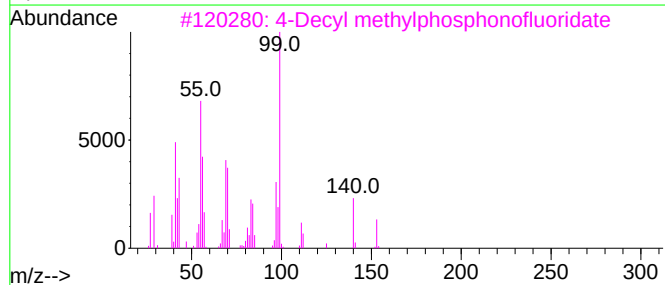
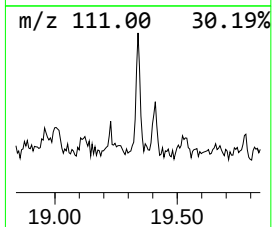
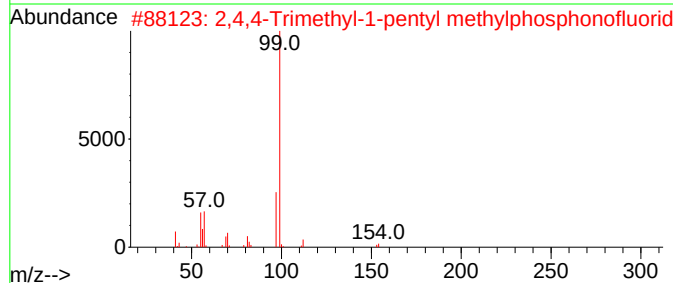
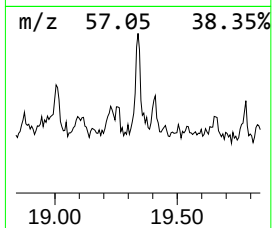
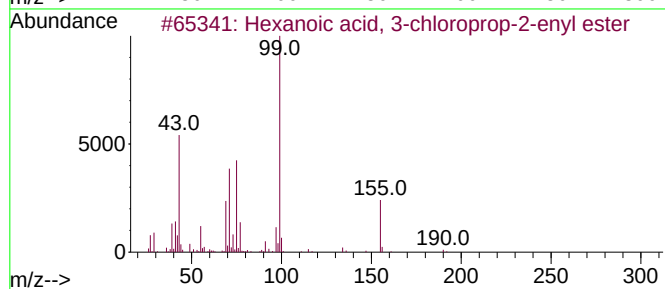
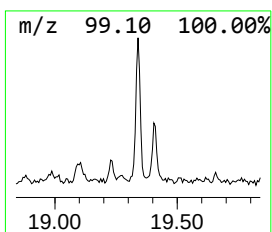
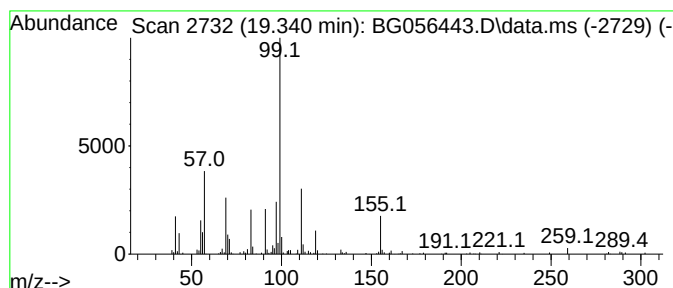
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown19.340 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.340	4.82 ng	126576	Phenanthrene-d10	17.648	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	47
2	2,4,4-Trimethyl-1-pentyl methylp...	210	C9H20FO2P	333416-06-1	47
3	4-Decyl methylphosphonofluoridate	238	C11H24FO2P	1000216-71-5	45
4	3,5,5-Trimethyl-1-hexyl methylph...	224	C10H22FO2P	1000298-44-9	38
5	Spiro[1,3-dioxolane-2,2'-[6,7]di...	182	C9H14N2O2	1000142-34-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
Acq On : 26 Jan 2023 15:05
Operator : CG/JU
Sample : 01289-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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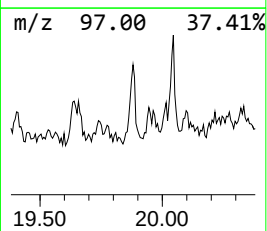
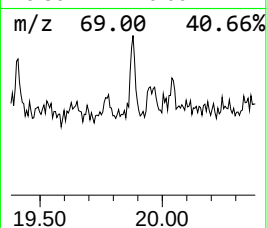
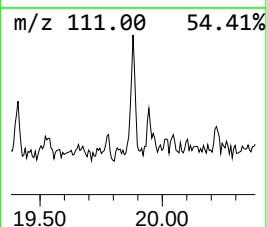
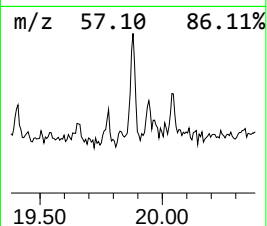
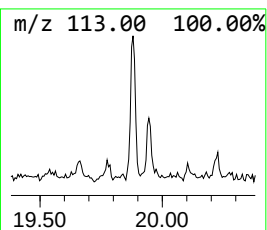
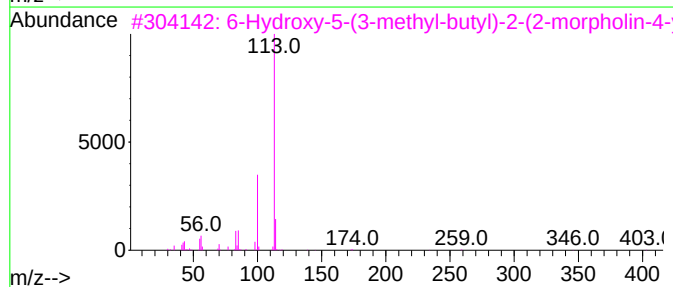
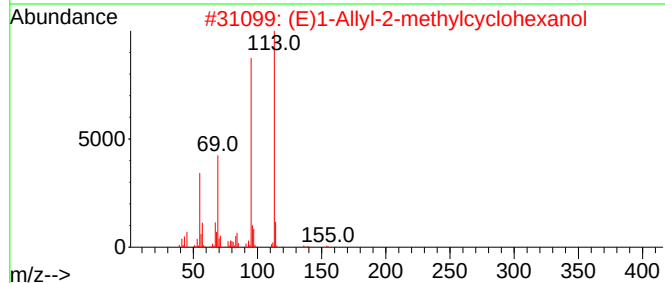
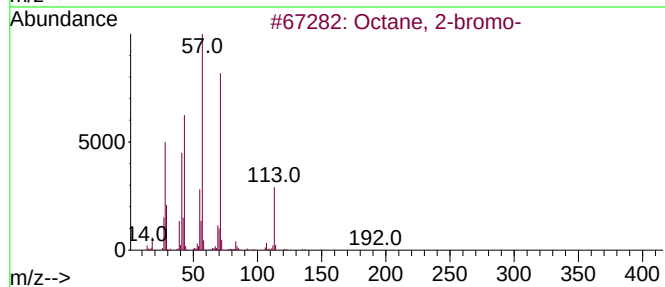
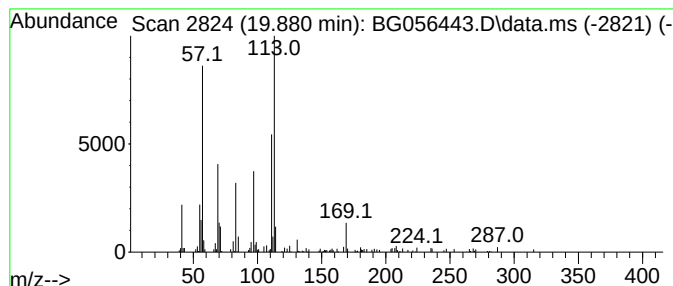
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown19.880 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.880	3.38 ng	110021	Chrysene-d12	21.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2-bromo-	192	C8H17Br	000557-35-7	43
2			(E)1-Allyl-2-methylcyclohexanol	154	C10H18O	1000311-73-7	38
3			6-Hydroxy-5-(3-methyl-butyl)-2-(...	403	C21H29N3O3S	1000317-62-4	35
4			1-Piperazinemethanol, 4-nonyl-	242	C14H30N2O	1000115-48-3	35
5			Pyrrolidine, 1-(3-methyl-1-oxohe...	337	C22H43NO	1000036-69-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
Acq On : 26 Jan 2023 15:05
Operator : CG/JU
Sample : 01289-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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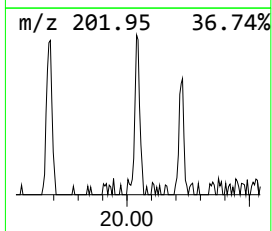
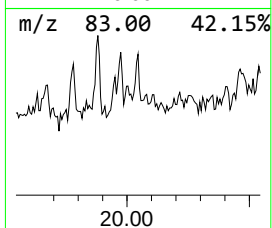
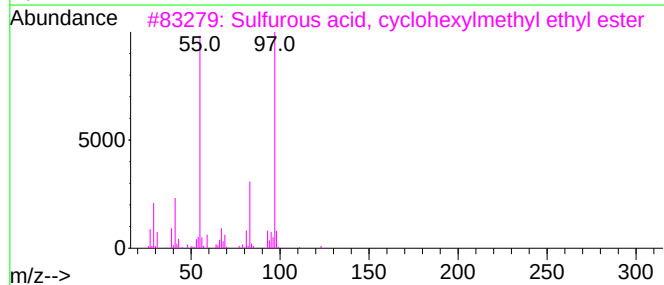
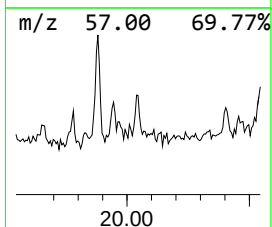
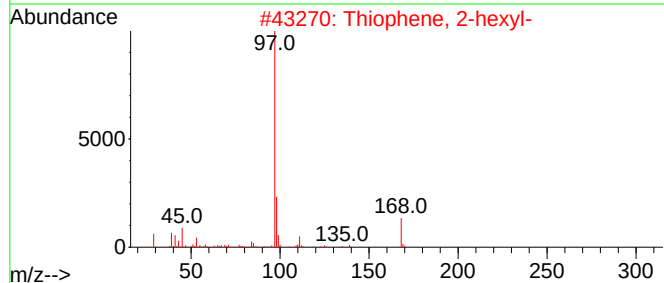
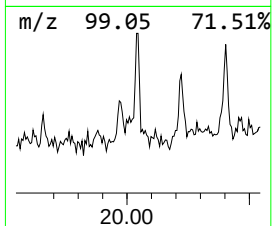
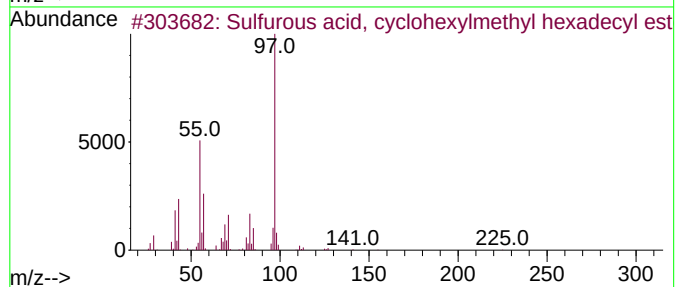
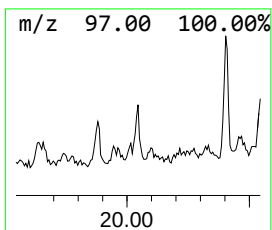
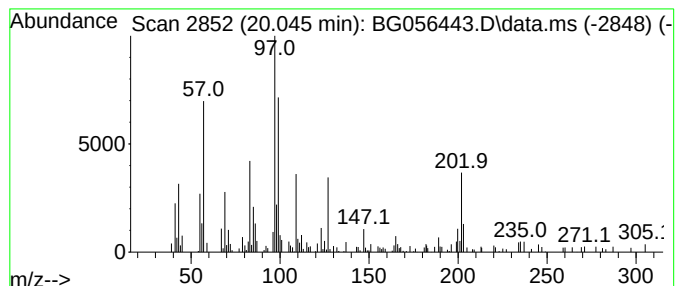
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown20.045 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.045	2.11 ng	68615	Chrysene-d12	21.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	27
2			Thiophene, 2-hexyl-	168	C10H16S	018794-77-9	27
3			Sulfurous acid, cyclohexylmethyl...	206	C9H18O3S	1000309-21-2	25
4			6-Undecyl-5,6-dihydro-2H-pyran-2...	252	C16H28O2	081017-06-3	22
5			3-(4-Methylpent-3-enyl)thiophene	166	C10H14S	062429-57-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
Acq On : 26 Jan 2023 15:05
Operator : CG/JU
Sample : 01289-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

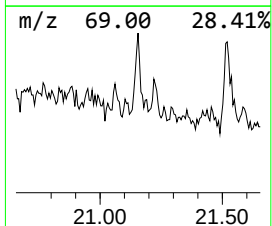
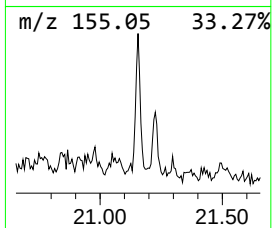
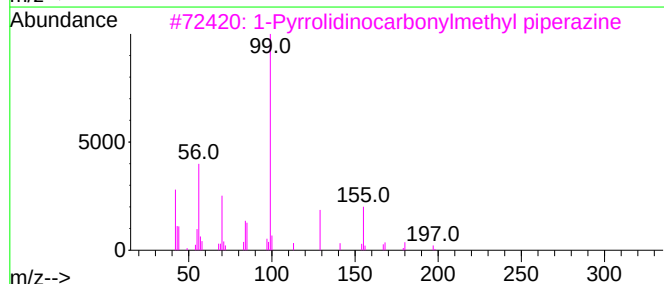
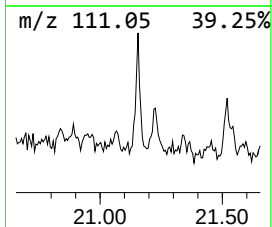
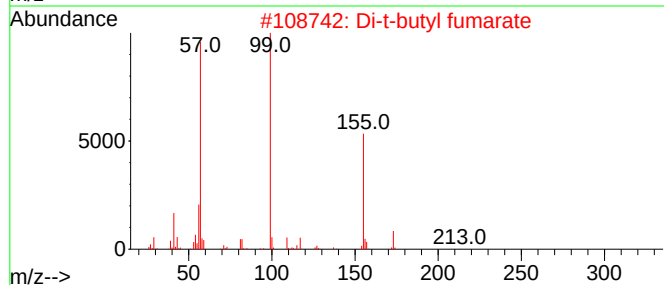
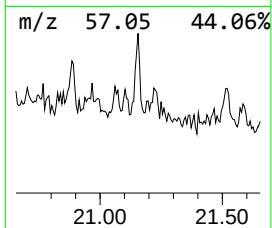
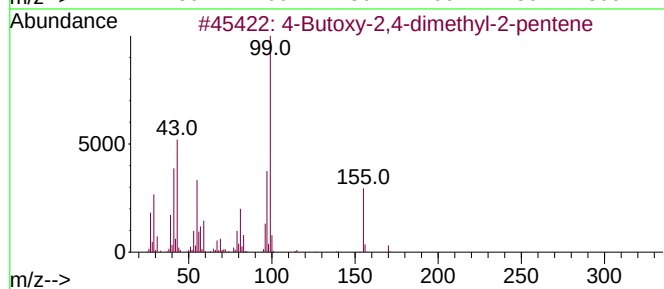
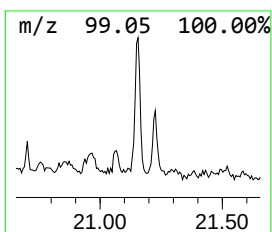
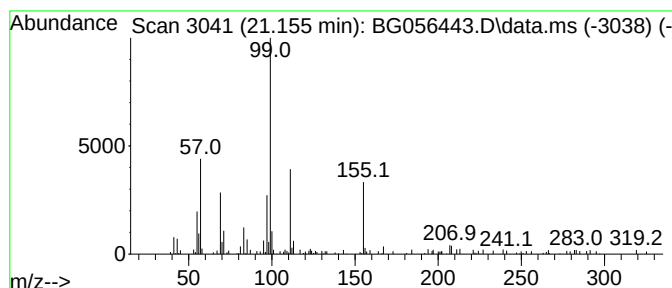
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 4-Butoxy-2,4-dimethyl-2-pen... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.155	2.30 ng	74885	Chrysene-d12	21.937	
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	47
3	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	43
4	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	43
5	2H-Pyran-2-one, tetrahydro-6-nonyl-	226	C14H26O2	002721-22-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
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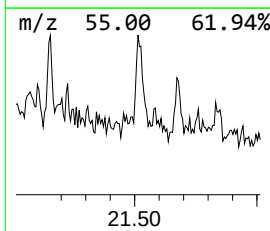
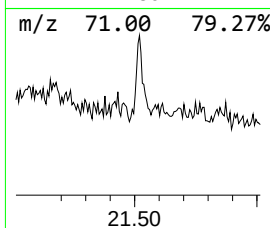
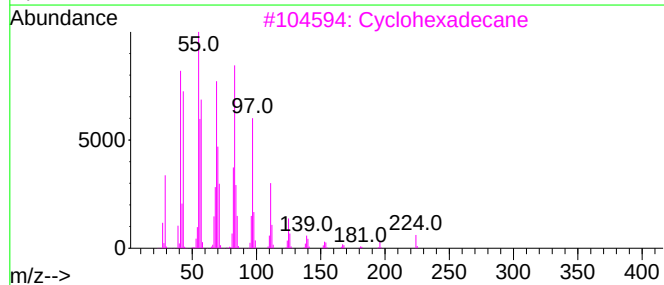
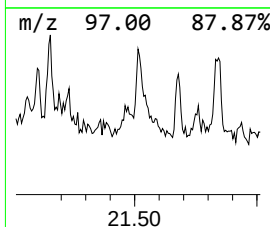
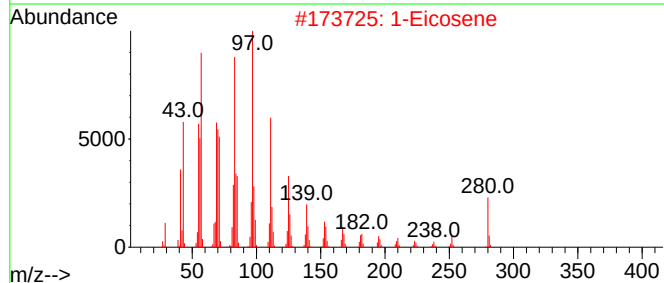
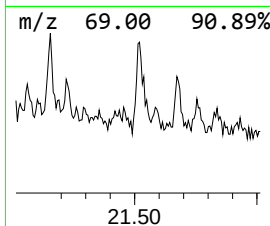
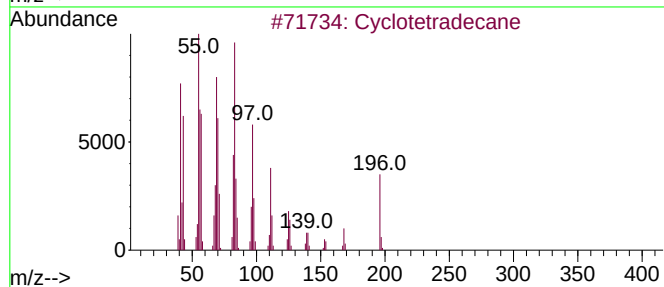
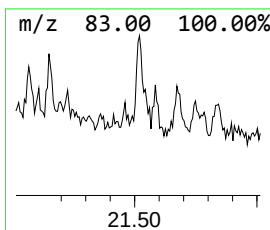
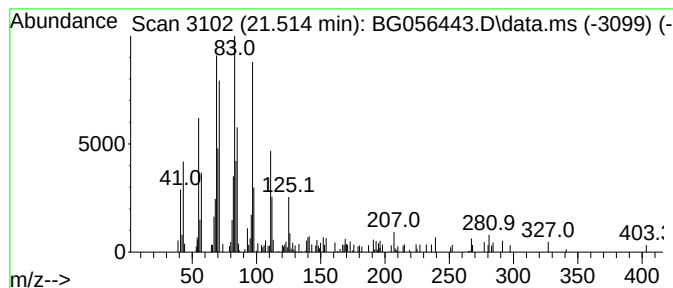
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Cyclotetradecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.514	3.13 ng	101765	Chrysene-d12	21.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	90
2			1-Eicosene	280	C20H40	003452-07-1	78
3			Cyclohexadecane	224	C16H32	000295-65-8	78
4			Dichloroacetic acid, 4-tetradecy...	324	C16H30Cl2O2	1000280-64-6	72
5			1-Octadecanol	270	C18H38O	000112-92-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
Acq On : 26 Jan 2023 15:05
Operator : CG/JU
Sample : 01289-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ209-STOCK

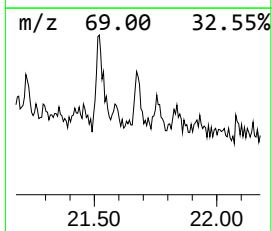
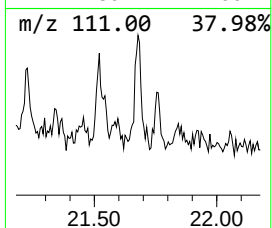
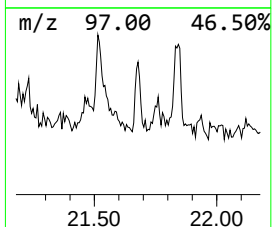
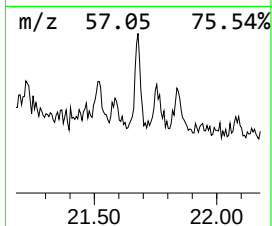
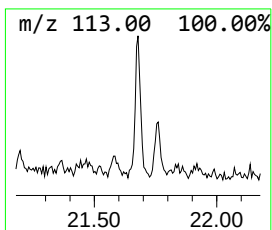
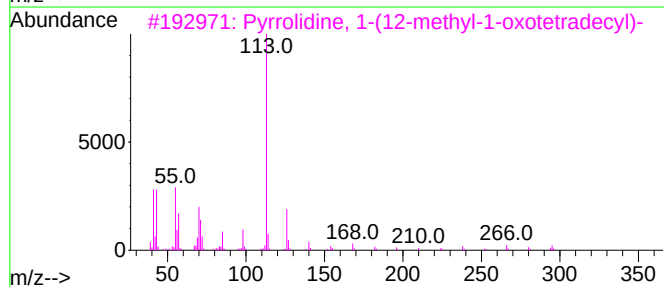
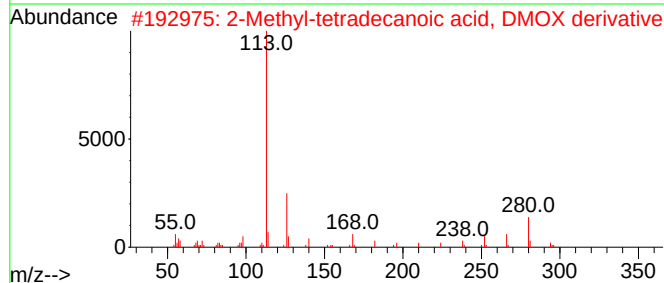
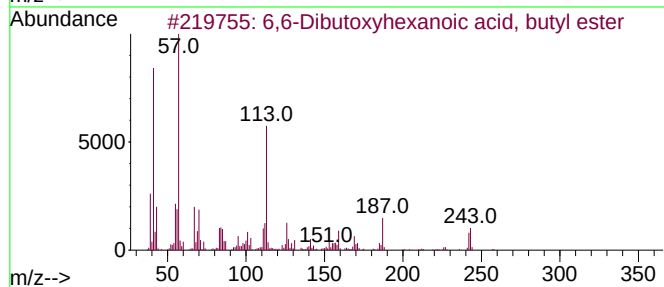
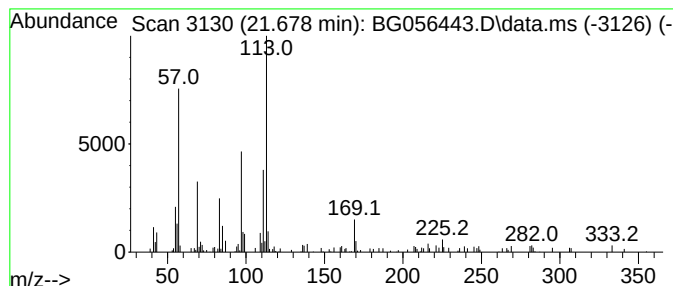
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown21.678 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.678	2.36 ng	76879	Chrysene-d12	21.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,6-Dibutoxyhexanoic acid, butyl...	316	C18H36O4	1000280-29-0	47		
2	2-Methyl-tetradecanoic acid, DMO...	295	C19H37NO	1000336-84-8	43		
3	Pyrrolidine, 1-(12-methyl-1-oxot...	295	C19H37NO	056630-61-6	43		
4	5,11,14-Eicostrienoic acid, pyrr...	359	C24H41NO	1000336-05-8	38		
5	11-Cyclopentylundecanoic acid, D...	307	C20H37NO	1000336-83-9	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012623\
Data File : BG056443.D
Acq On : 26 Jan 2023 15:05
Operator : CG/JU
Sample : 01289-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ209-STOCK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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
2-Pentanone, 4-...	5.333	17.2	ng	140005	1	8.294	162870	20.0
Fumaric acid, d...	13.940	3.6	ng	77437	3	14.910	430072	20.0
unknown14.833	14.833	2.3	ng	48424	3	14.910	430072	20.0
2-Propionyl-6-m...	15.809	4.8	ng	102685	3	14.910	430072	20.0
Benzophenone	16.249	13.5	ng	289807	3	14.910	430072	20.0
Dodecyl isobuty...	16.860	2.3	ng	59897	4	17.648	524871	20.0
4-Decyl methylp...	17.007	6.8	ng	177213	4	17.648	524871	20.0
unknown17.078	17.078	2.5	ng	66161	4	17.648	524871	20.0
unknown17.759	17.759	2.3	ng	61482	4	17.648	524871	20.0
2,4,4,6,6,8,8-H...	18.400	4.5	ng	118339	4	17.648	524871	20.0
unknown18.552	18.552	2.7	ng	70106	4	17.648	524871	20.0
Benzene, (1-met...	18.970	8.4	ng	220839	4	17.648	524871	20.0
Thiophene, 2-he...	19.005	3.2	ng	82945	4	17.648	524871	20.0
unknown19.340	19.340	4.8	ng	126576	4	17.648	524871	20.0
unknown19.880	19.880	3.4	ng	110021	5	21.937	650980	20.0
unknown20.045	20.045	2.1	ng	68615	5	21.937	650980	20.0
4-Butoxy-2,4-di...	21.155	2.3	ng	74885	5	21.937	650980	20.0
Cyclotetradecane	21.514	3.1	ng	101765	5	21.937	650980	20.0
unknown21.678	21.678	2.4	ng	76879	5	21.937	650980	20.0