

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
 Data File : BG061226.D
 Acq On : 16 May 2024 18:42
 Operator : MA/JU
 Sample : P2477-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ETGI-339

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-BG043024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061226.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.073	9	14	18	rBV4	8713	19353	1.29%	0.169%
2	3.149	22	27	40	rVB	260317	427155	28.50%	3.727%
3	3.672	111	116	124	rBV	41095	63398	4.23%	0.553%
4	5.523	425	431	442	rBV	389513	610980	40.76%	5.331%
5	7.109	691	701	712	rBV	411822	697625	46.54%	6.087%
6	7.932	833	841	847	rBV	111083	188297	12.56%	1.643%
7	9.083	1028	1037	1044	rBV	258702	451856	30.14%	3.943%
8	9.635	1125	1131	1138	rVB4	9869	16695	1.11%	0.146%
9	10.487	1270	1276	1288	rBV	44146	78655	5.25%	0.686%
10	10.722	1308	1316	1323	rBV	147824	257455	17.17%	2.246%
11	10.863	1332	1340	1346	rVB3	11016	21383	1.43%	0.187%
12	11.463	1436	1442	1452	rVB3	14790	28445	1.90%	0.248%
13	13.178	1725	1734	1743	rBV	672764	1038183	69.26%	9.059%
14	14.559	1962	1969	1974	rBV	234116	375004	25.02%	3.272%
15	14.618	1974	1979	1984	rVB4	9002	16109	1.07%	0.141%
16	14.753	1998	2002	2003	rBV2	16044	16122	1.08%	0.141%
17	16.051	2216	2223	2240	rBV	571727	916085	61.11%	7.993%
18	16.275	2254	2261	2262	rBV4	16284	26964	1.80%	0.235%
19	16.968	2373	2379	2386	rBV8	28843	60277	4.02%	0.526%
20	17.062	2389	2395	2399	rVV2	24125	39683	2.65%	0.346%
21	17.121	2399	2405	2411	rVV3	19539	36634	2.44%	0.320%
22	17.303	2430	2436	2441	rBV	288936	459339	30.64%	4.008%
23	17.344	2441	2443	2450	rVB	51044	71370	4.76%	0.623%
24	17.438	2455	2459	2465	rVV	27905	38309	2.56%	0.334%
25	17.491	2465	2468	2474	rBV8	15659	26649	1.78%	0.233%
26	17.802	2518	2521	2523	rBV3	13752	18063	1.20%	0.158%
27	18.208	2586	2590	2599	rVB2	57506	110611	7.38%	0.965%
28	18.378	2616	2619	2623	rVB3	23828	32816	2.19%	0.286%
29	18.496	2636	2639	2644	rBV3	23775	28858	1.93%	0.252%
30	19.054	2732	2734	2737	rBV3	22722	23563	1.57%	0.206%
31	19.148	2747	2750	2755	rVB5	56991	67387	4.50%	0.588%
32	19.242	2762	2766	2772	rBV	68222	92622	6.18%	0.808%
33	19.359	2782	2786	2792	rVB	315281	439854	29.34%	3.838%
34	19.465	2801	2804	2814	rBV8	36364	106711	7.12%	0.931%
35	19.724	2839	2848	2857	rBV	470763	854269	56.99%	7.454%
36	19.923	2877	2882	2887	rBV	1169514	1499024	100.00%	13.080%

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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-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.563	3155	3161	3166	rBV3	347891	875874	58.43%	7.642%
38	21.610	3167	3169	3182	rVB	297958	507904	33.88%	4.432%
39	23.707	3521	3526	3532	rBV	143836	336559	22.45%	2.937%
40	24.694	3686	3694	3701	rBV	180787	484475	32.32%	4.227%

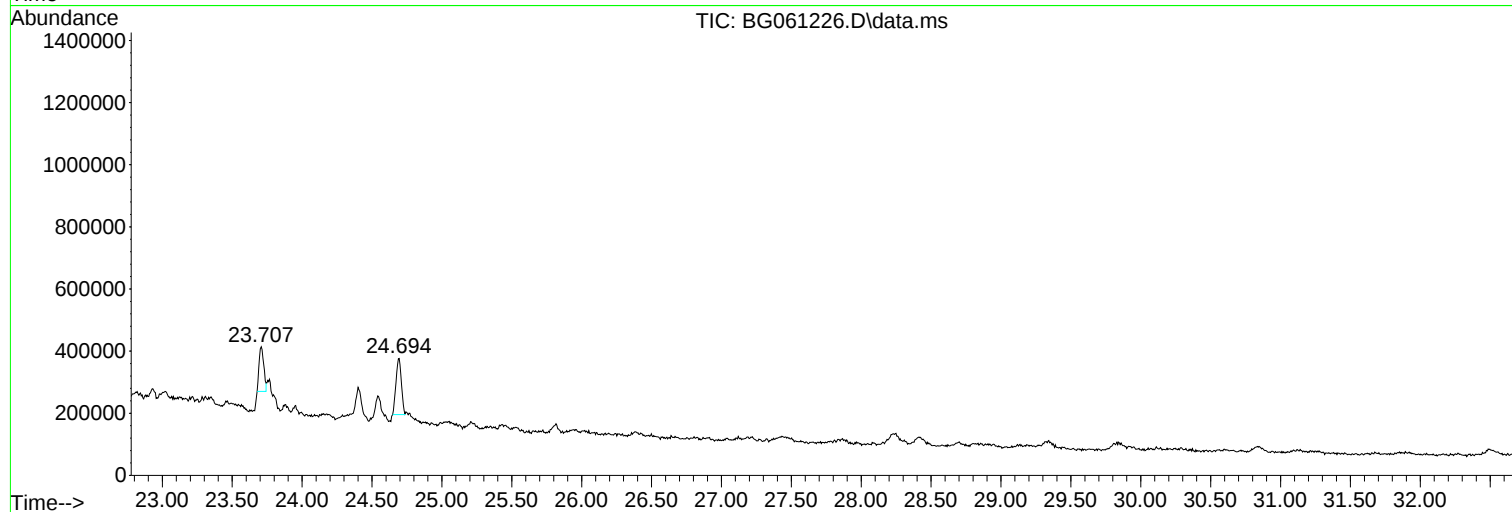
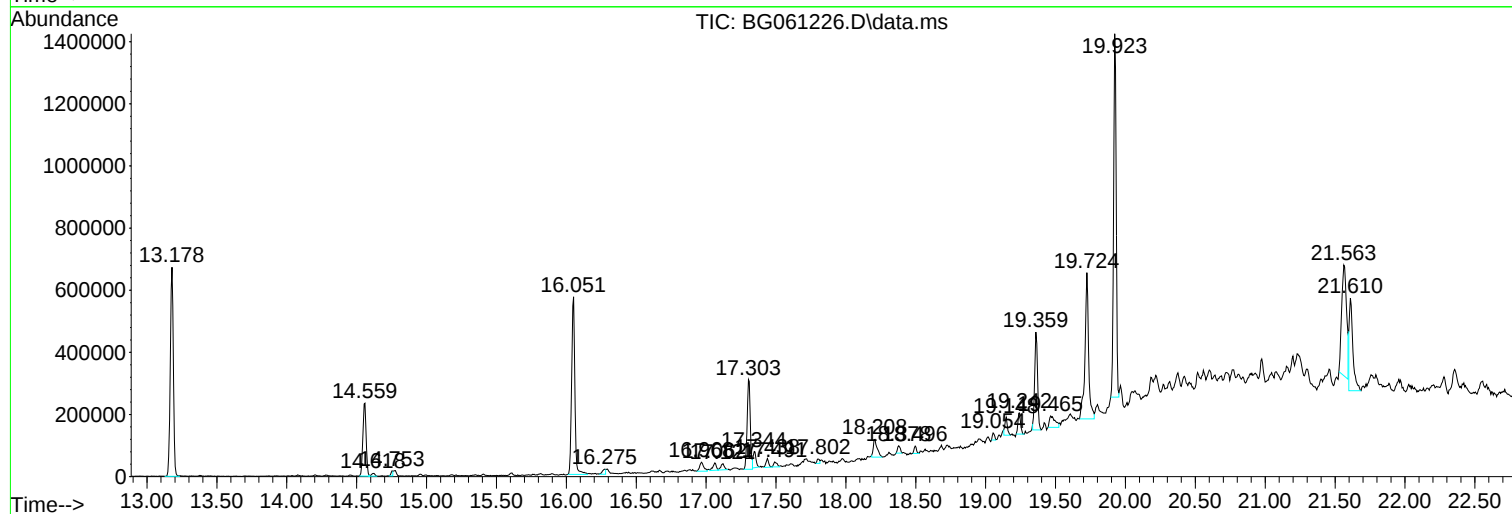
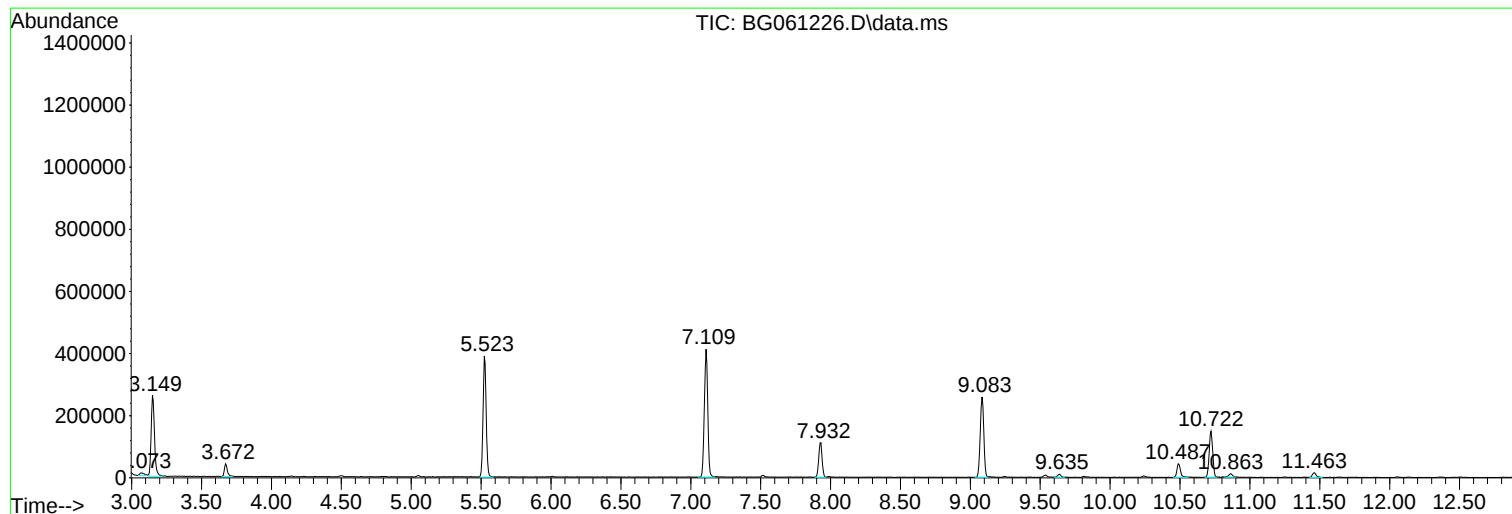
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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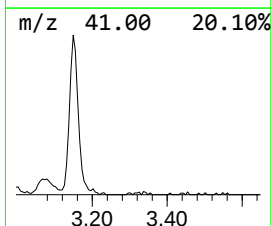
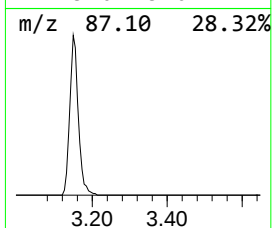
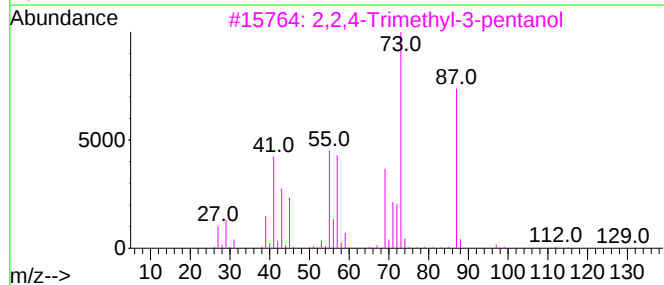
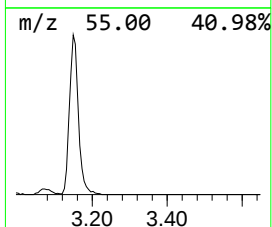
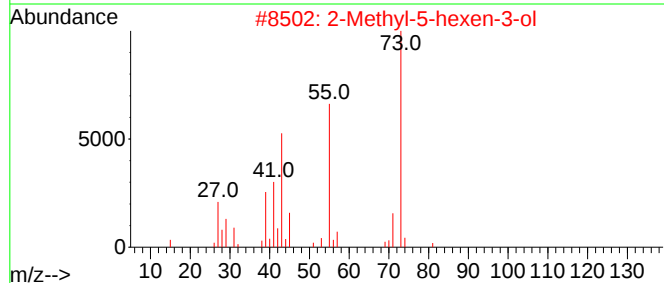
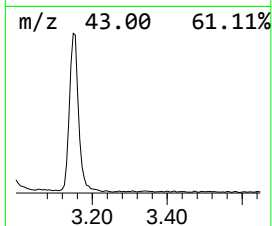
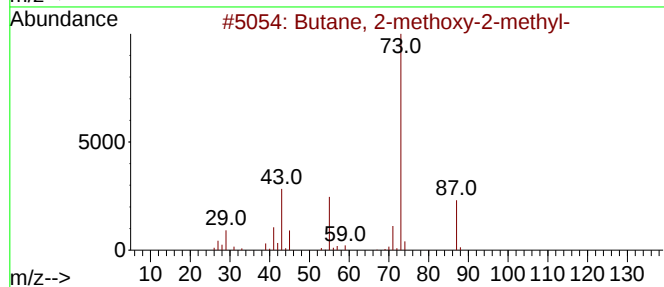
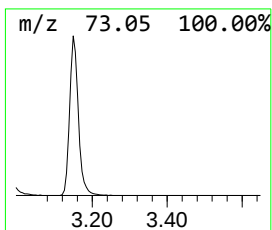
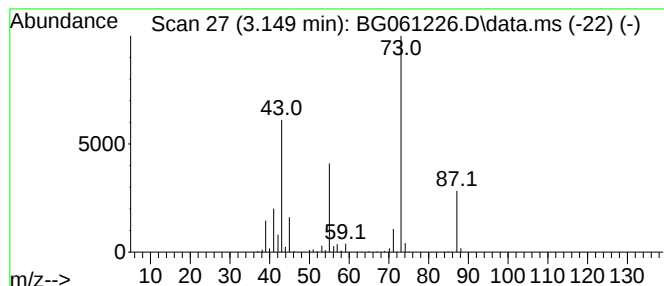
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.149	45.37 ng	427155	1,4-Dichlorobenzene-d4	7.932

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
5			1-Propene-1-thiol	74	C3H6S	000925-89-3	17



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ClientSampleId :
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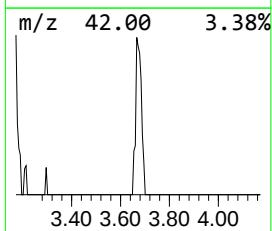
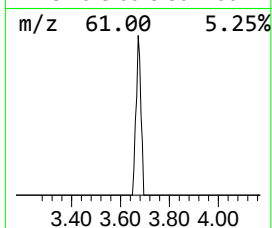
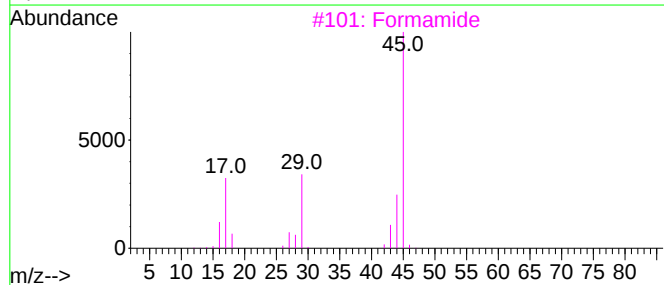
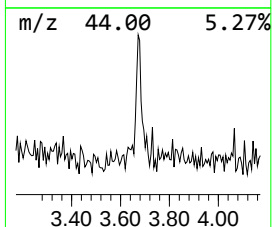
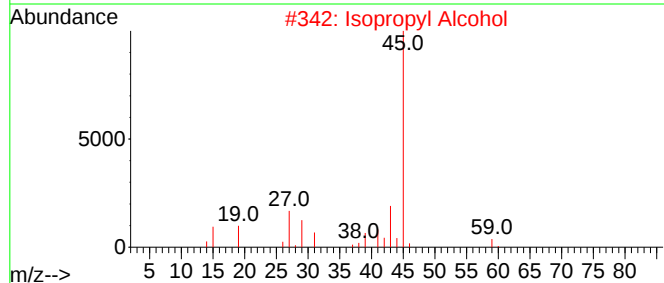
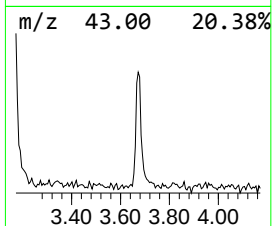
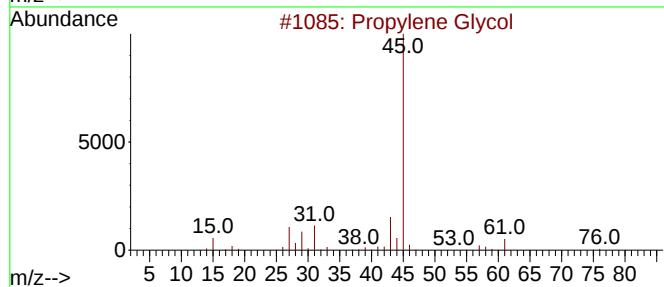
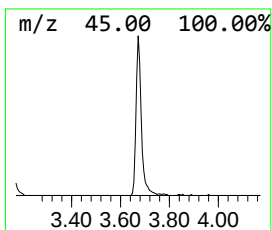
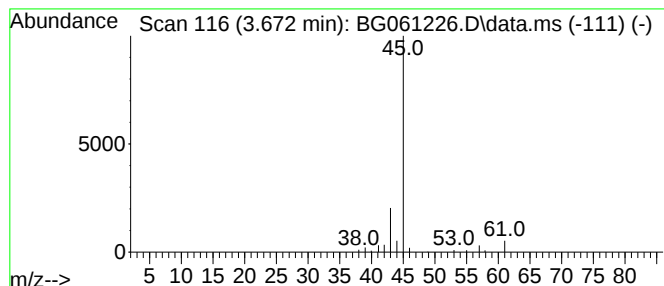
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown3.672 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.672	6.73 ng	63398	1,4-Dichlorobenzene-d4	7.932

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	9
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3			Formamide	45	CH3NO	000075-12-7	5
4			L-Lactic acid	90	C3H6O3	000079-33-4	4
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	4



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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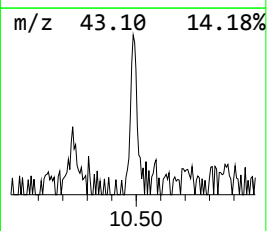
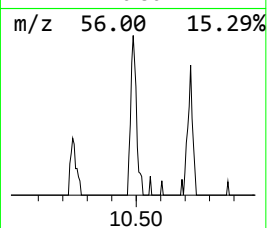
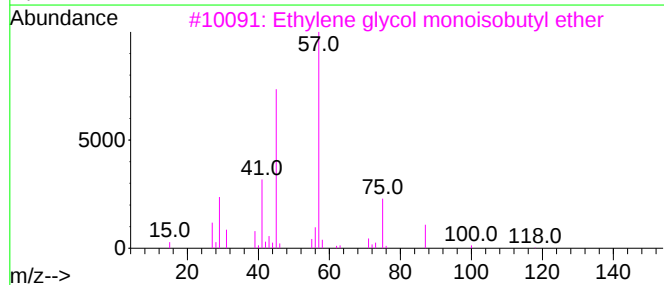
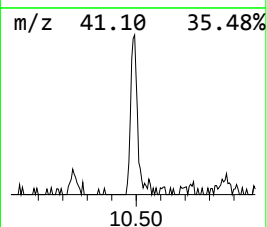
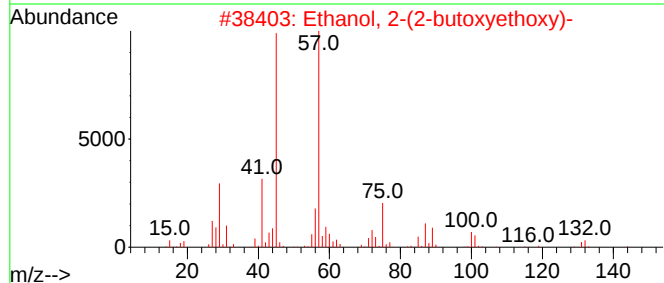
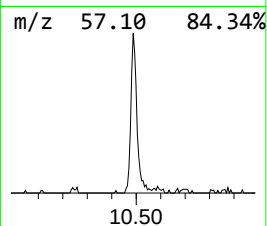
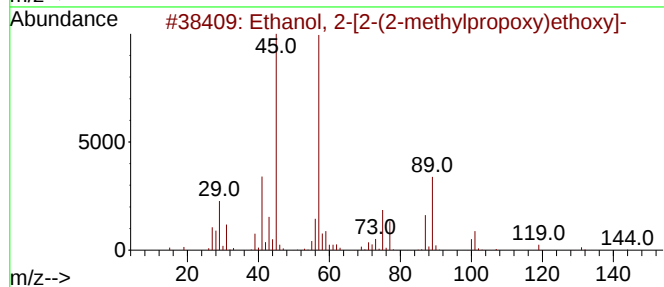
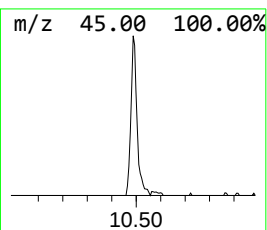
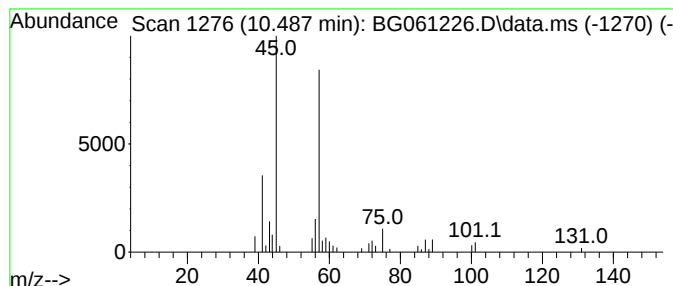
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-[2-(2-methylprop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.487	6.11 ng	78655	Naphthalene-d8	10.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	56
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
4			Triethylene glycol	150	C6H14O4	000112-27-6	50
5			Butane, 1-methoxy-	88	C5H12O	000628-28-4	47



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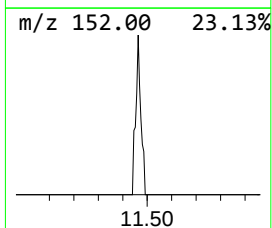
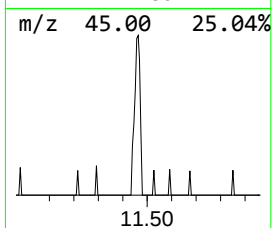
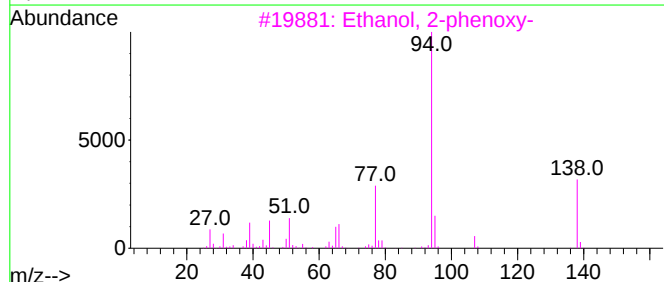
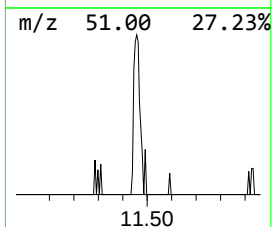
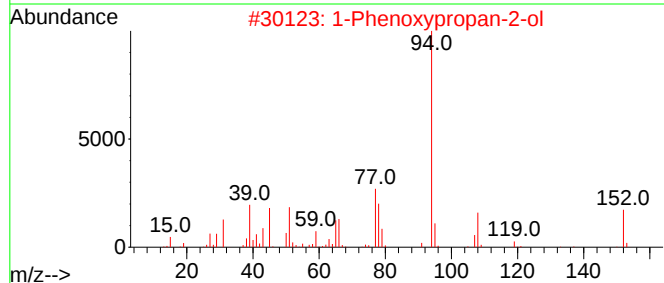
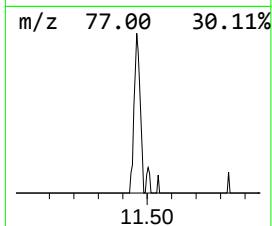
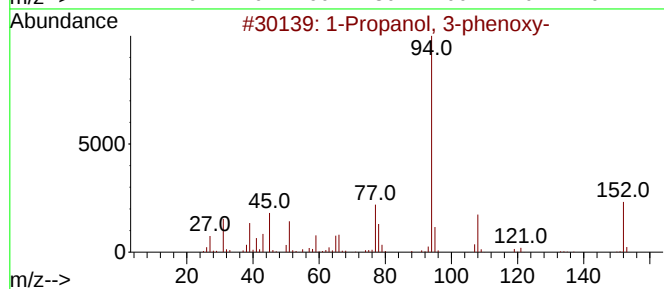
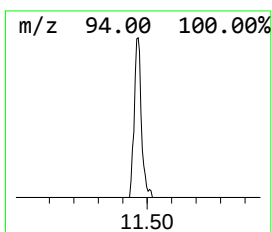
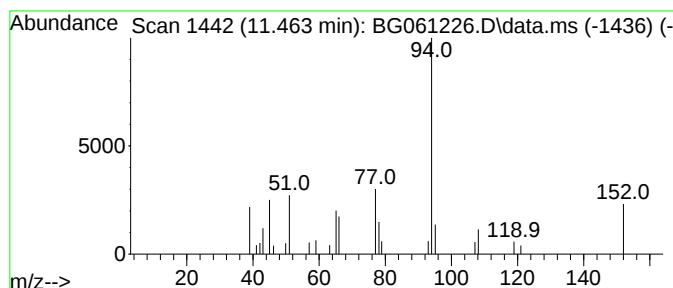
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Propanol, 3-phenoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.463	2.21 ng	28445	Naphthalene-d8	10.722	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	81
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	80
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	butanedioic acid, monophenyl ester	194	C10H10O4	1000400-29-4	53
5	Oxirane, (phenoxyethyl)-	150	C9H10O2	000122-60-1	47



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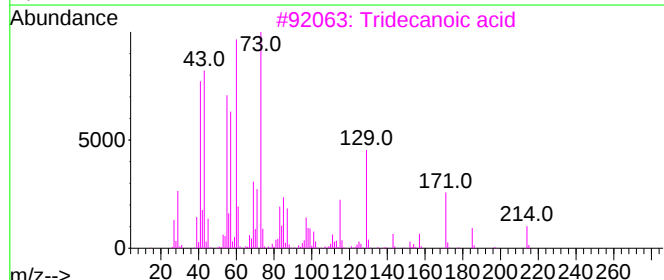
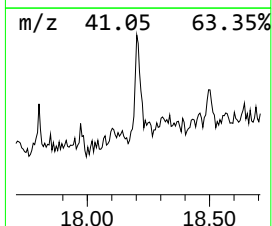
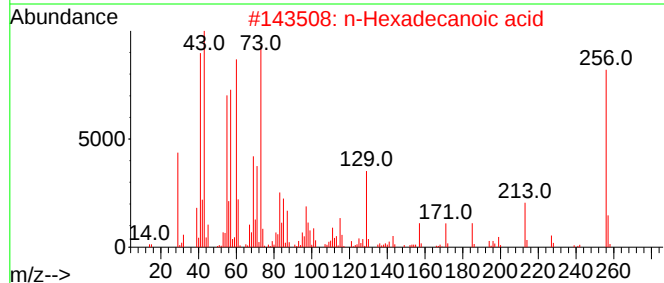
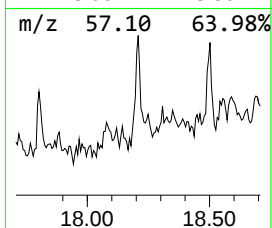
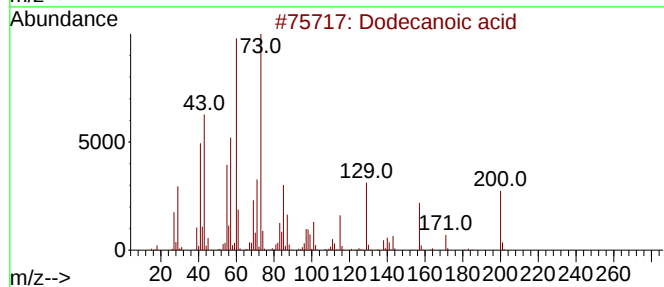
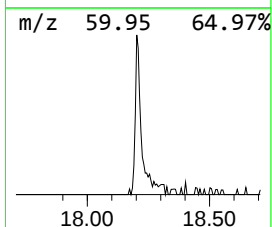
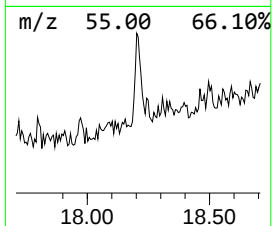
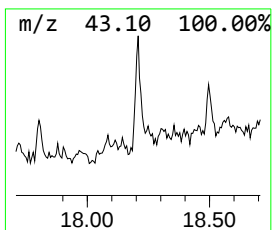
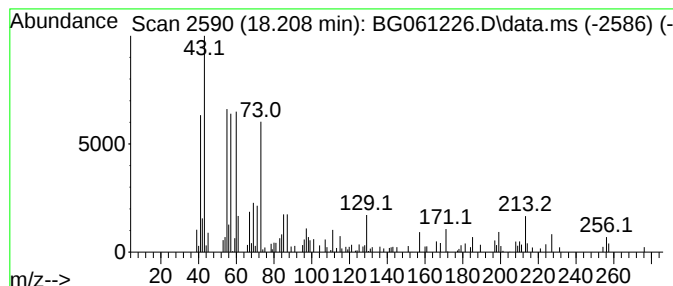
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.208	4.82 ng	110611	Phenanthrene-d10	17.303

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	90
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
3			Tridecanoic acid	214	C13H26O2	000638-53-9	78
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5			n-Decanoic acid	172	C10H20O2	000334-48-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061226.D
Acq On : 16 May 2024 18:42
Operator : MA/JU
Sample : P2477-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ETGI-339

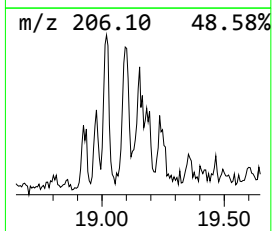
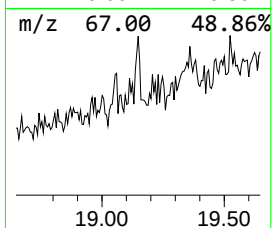
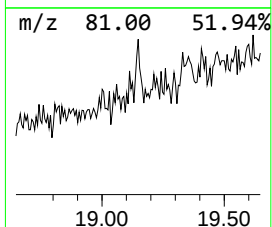
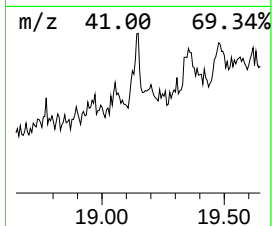
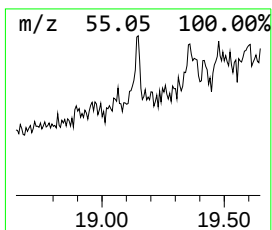
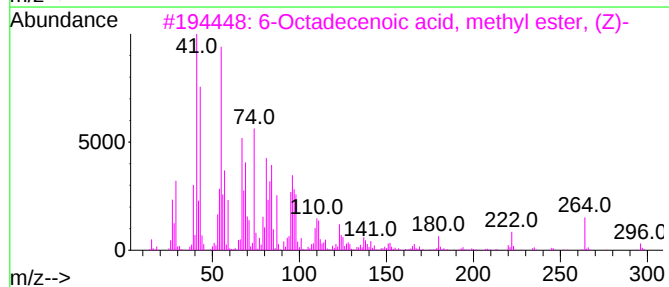
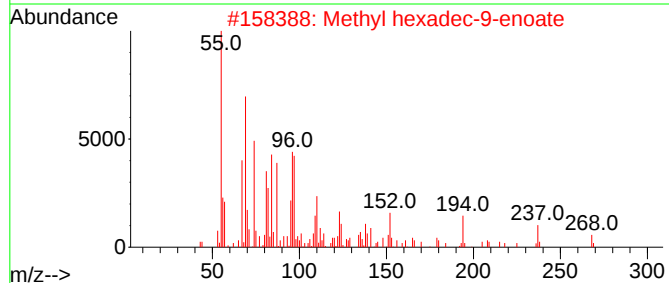
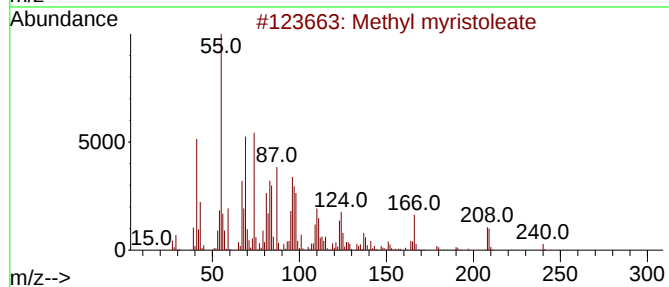
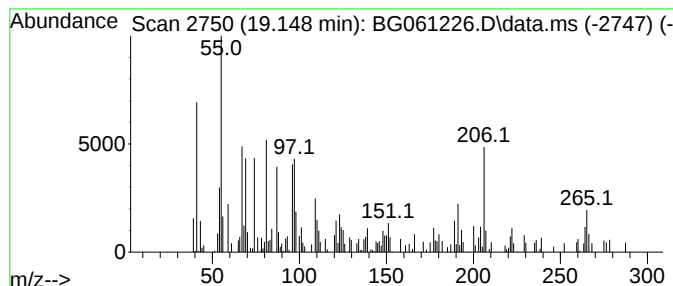
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown19.148 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.148	2.93 ng	67387	Phenanthrene-d10	17.303

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl myristoleate	240	C15H28O2	056219-06-8	35
2			Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	35
3			6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	27
4			Oxiraneundecanoic acid, 3-pentyl...	312	C19H36O3	038520-30-8	27
5			Z,Z-3,13-Octadecadien-1-ol	266	C18H34O	1000131-10-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061226.D
Acq On : 16 May 2024 18:42
Operator : MA/JU
Sample : P2477-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ETGI-339

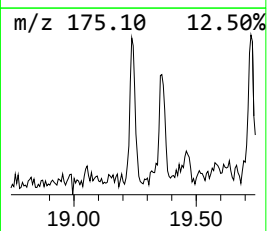
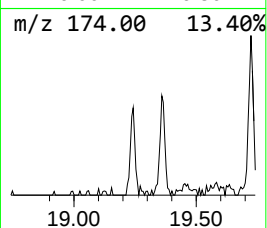
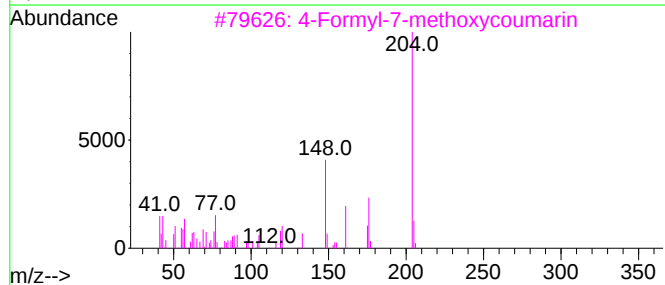
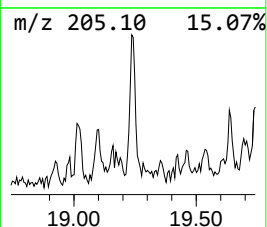
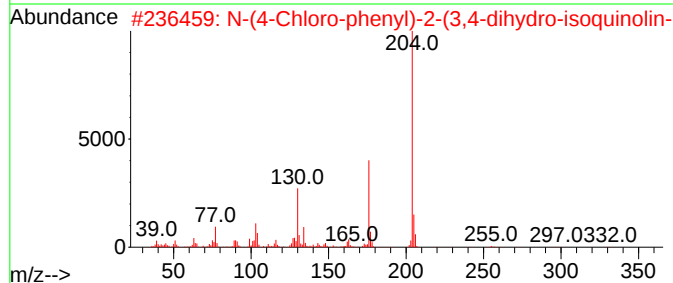
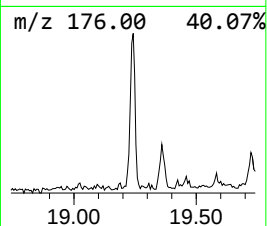
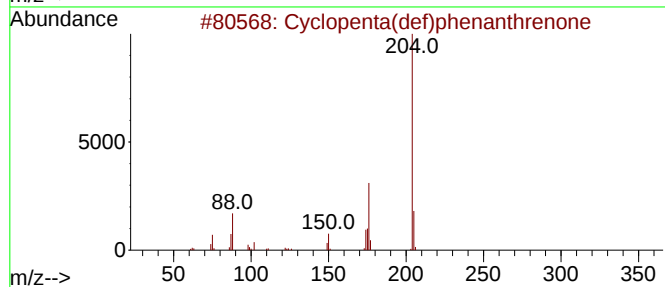
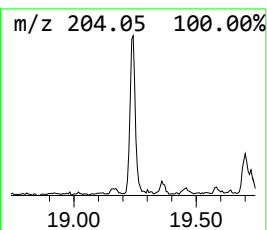
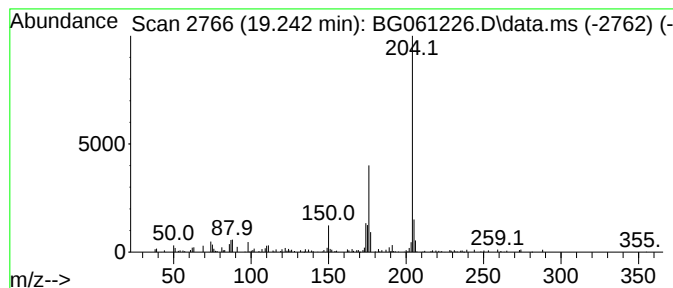
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclopenta(def)phenanthrenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.242	4.03 ng	92622	Phenanthrene-d10	17.303

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	86
2			N-(4-Chloro-phenyl)-2-(3,4-dihyd...	330	C17H15ClN2OS	1010296-34-3	50
3			4-Formyl-7-methoxycoumarin	204	C11H8O4	1000429-03-0	49
4			[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	49
5			3-(4-Fluorophenoxy)phenol	204	C12H9FO2	025967-60-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061226.D
Acq On : 16 May 2024 18:42
Operator : MA/JU
Sample : P2477-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ETGI-339

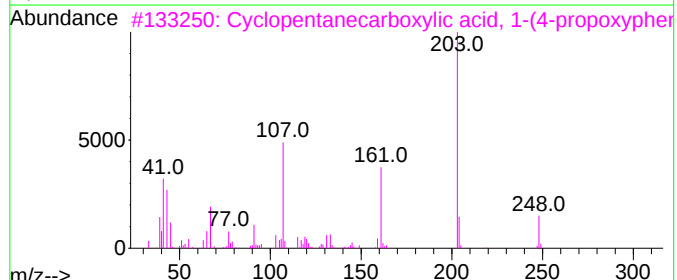
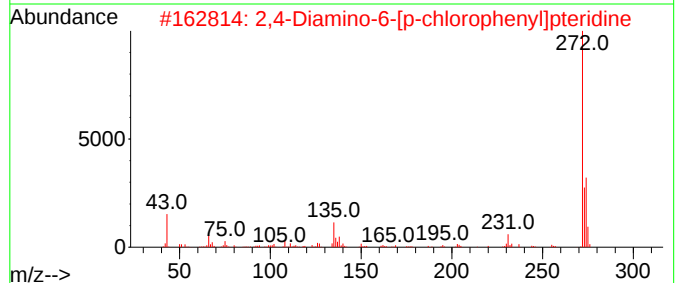
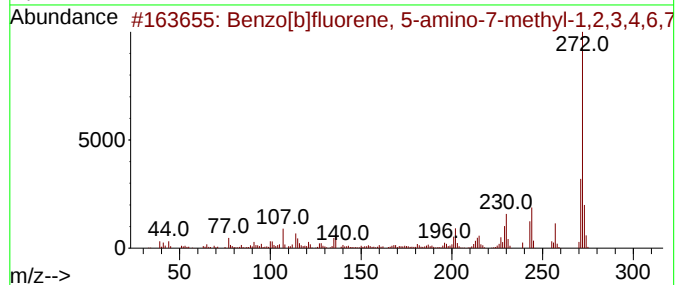
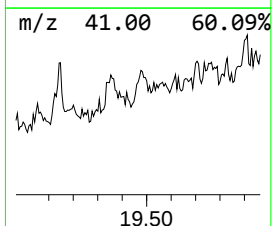
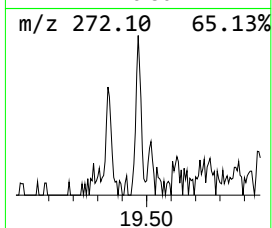
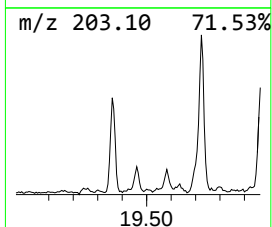
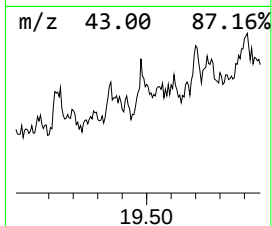
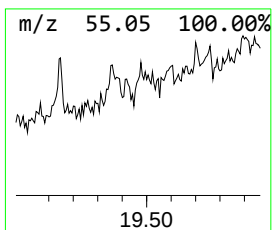
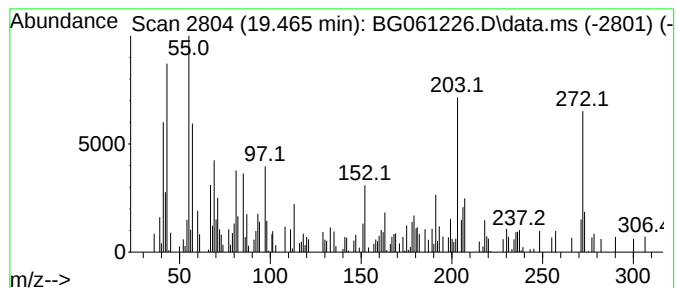
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown19.465 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.465	2.44 ng	106711	Chrysene-d12	21.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluorene, 5-amino-7-meth...	272	C16H20N2S	1000310-69-7	18
2			2,4-Diamino-6-[p-chlorophenyl]pt...	272	C12H9ClN6	030146-32-8	11
3			Cyclopentanecarboxylic acid, 1-(...	248	C15H20O3	074316-95-3	11
4			Biphenyl-4-yl-p-tolyl-methanone	272	C20H16O	039148-55-5	11
5			Estradiol	272	C18H24O2	000050-28-2	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061226.D
Acq On : 16 May 2024 18:42
Operator : MA/JU
Sample : P2477-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ETGI-339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.149	45.4	ng	427155	1	7.932	188297	20.0
unknown3.672	3.672	6.7	ng	63398	1	7.932	188297	20.0
Ethanol, 2-[2-(...	10.487	6.1	ng	78655	2	10.722	257455	20.0
1-Propanol, 3-p...	11.463	2.2	ng	28445	2	10.722	257455	20.0
Dodecanoic acid	18.208	4.8	ng	110611	4	17.303	459339	20.0
unknown19.148	19.148	2.9	ng	67387	4	17.303	459339	20.0
Cyclopenta(def)...	19.242	4.0	ng	92622	4	17.303	459339	20.0
unknown19.465	19.465	2.4	ng	106711	5	21.569	875874	20.0