

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040125\
 Data File : BG064133.D
 Acq On : 1 Apr 2025 13:43
 Operator : RC/JU
 Sample : Q1672-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-8

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-BG030525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG064133.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.986	315	323	330	rBV2	79806	121889	4.68%	0.914%
2	5.450	393	402	412	rBV	612531	971127	37.29%	7.282%
3	7.025	663	670	680	rBV	681277	1133160	43.51%	8.497%
4	7.859	806	812	820	rVB2	142602	232574	8.93%	1.744%
5	9.011	1000	1008	1017	rBV	402021	696349	26.74%	5.221%
6	10.644	1279	1286	1294	rBV	181610	320632	12.31%	2.404%
7	13.106	1698	1705	1712	rBV	1045145	1589946	61.05%	11.922%
8	14.481	1931	1939	1946	rVB	293956	450191	17.29%	3.376%
9	15.838	2164	2170	2177	rBV	250229	362796	13.93%	2.720%
10	15.967	2186	2192	2201	rBV	929139	1409907	54.14%	10.572%
11	16.402	2261	2266	2274	rVB	25272	39022	1.50%	0.293%
12	17.225	2399	2406	2411	rBV	375468	578582	22.22%	4.338%
13	17.612	2466	2472	2480	rBV4	33364	50315	1.93%	0.377%
14	18.558	2629	2633	2639	rVB3	27152	37612	1.44%	0.282%
15	18.970	2698	2703	2711	rVB7	16799	36877	1.42%	0.277%
16	19.551	2798	2802	2809	rBV	40873	50932	1.96%	0.382%
17	19.845	2845	2852	2858	rBV	1935249	2604220	100.00%	19.527%
18	20.533	2961	2969	2982	rBV	656095	918970	35.29%	6.891%
19	20.644	2984	2988	2993	rVB7	15670	27769	1.07%	0.208%
20	21.132	3067	3071	3079	rVB	140028	196096	7.53%	1.470%
21	21.449	3119	3125	3133	rBV	420573	692581	26.59%	5.193%
22	22.254	3257	3262	3266	rVB7	14182	27602	1.06%	0.207%
23	24.463	3629	3638	3649	rBV3	257332	707782	27.18%	5.307%
24	29.299	4453	4461	4463	rBV8	36638	79314	3.05%	0.595%

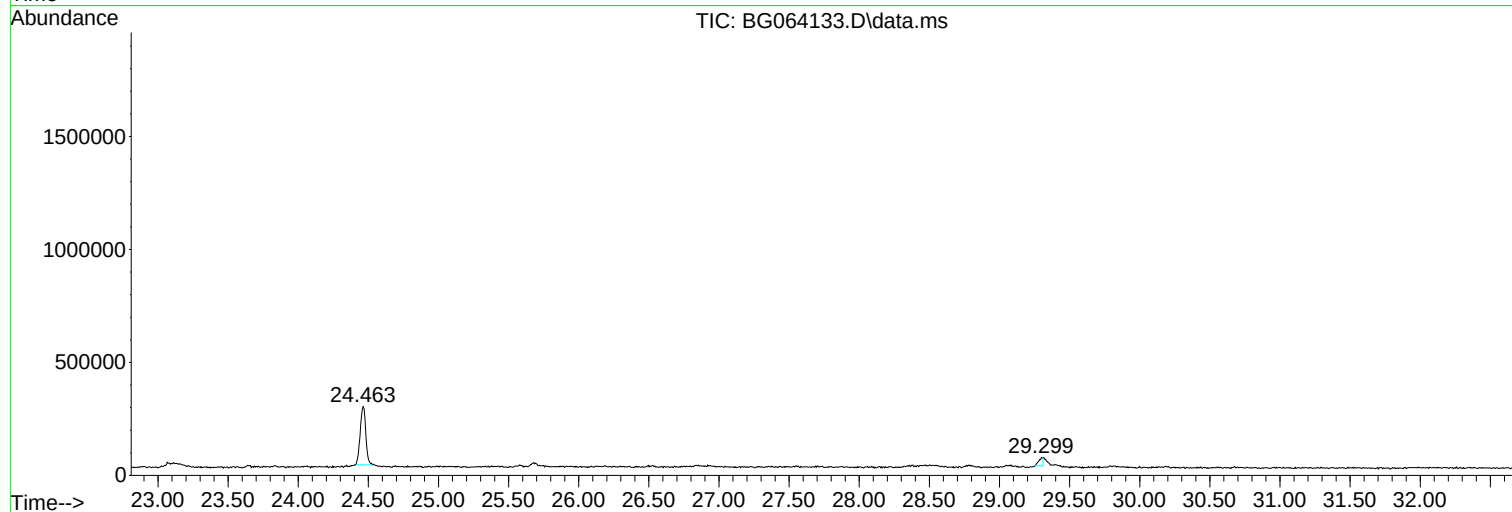
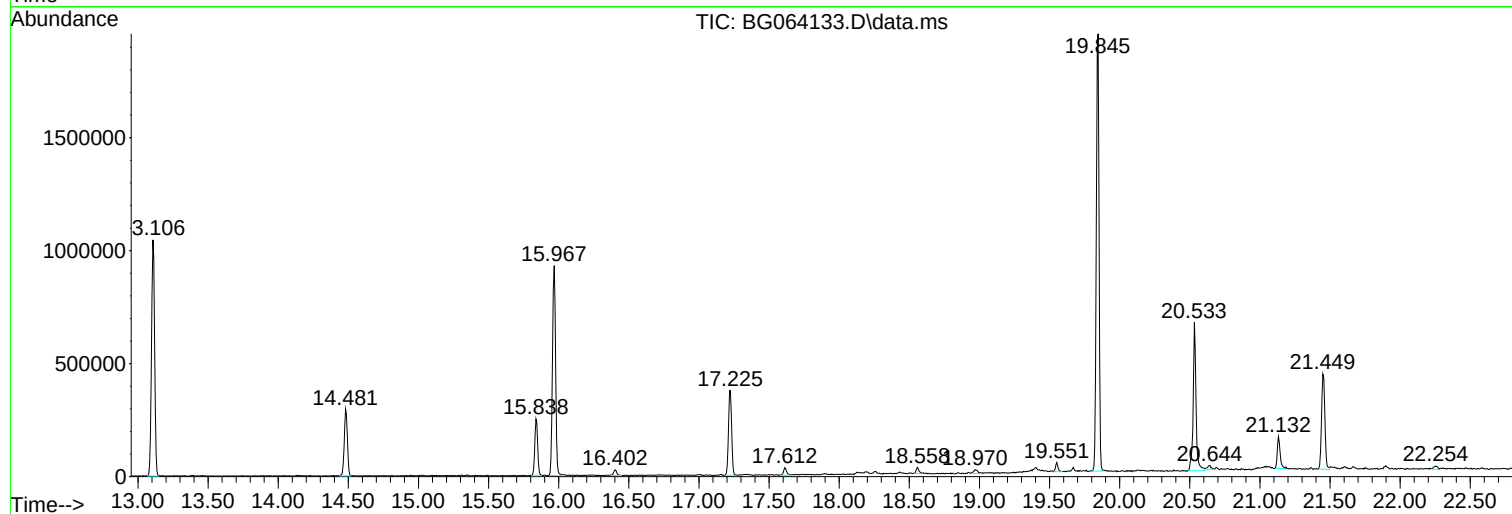
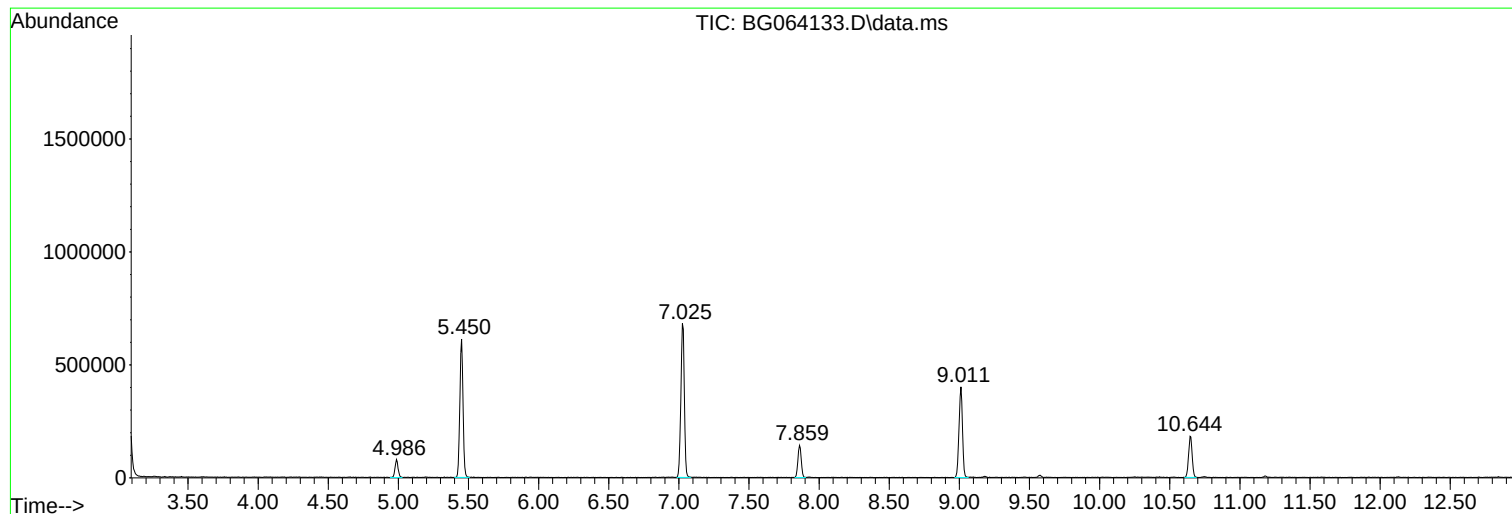
Sum of corrected areas: 13336245

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040125\
Data File : BG064133.D
Acq On : 1 Apr 2025 13:43
Operator : RC/JU
Sample : Q1672-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040125\
Data File : BG064133.D
Acq On : 1 Apr 2025 13:43
Operator : RC/JU
Sample : Q1672-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-8

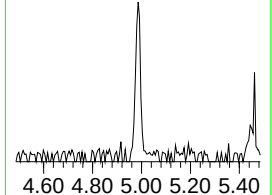
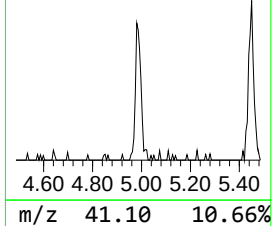
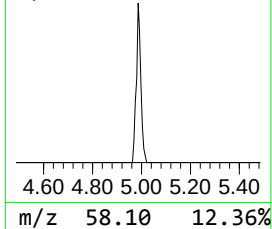
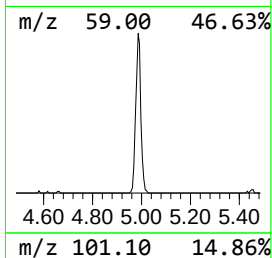
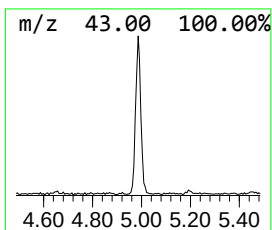
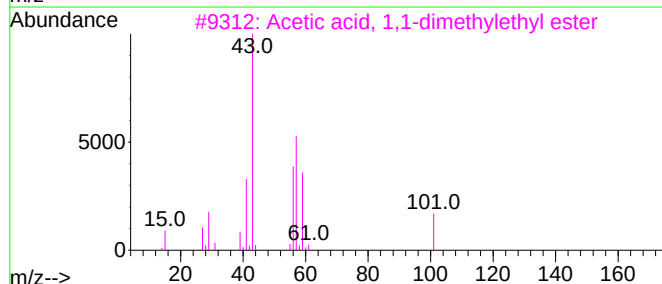
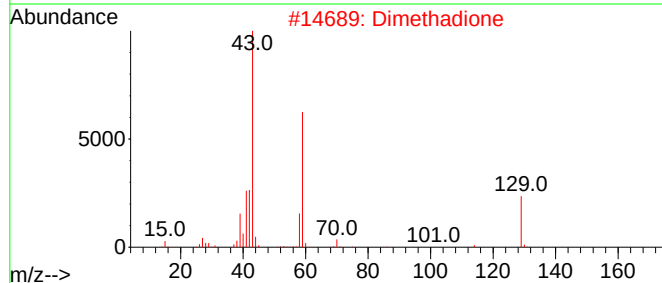
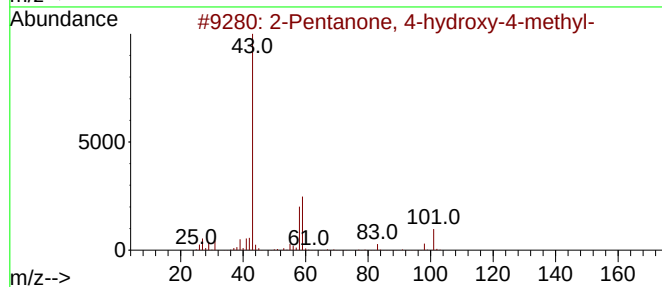
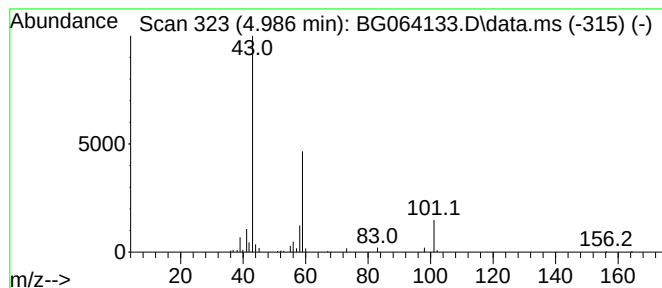
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.986	10.48 ng	121889	1,4-Dichlorobenzene-d4	7.859

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Dimethadione	129	C5H7NO3	000695-53-4	45		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
5	3-Nonyl acetate	186	C11H22O2	1010429-16-2	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040125\
Data File : BG064133.D
Acq On : 1 Apr 2025 13:43
Operator : RC/JU
Sample : Q1672-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-8

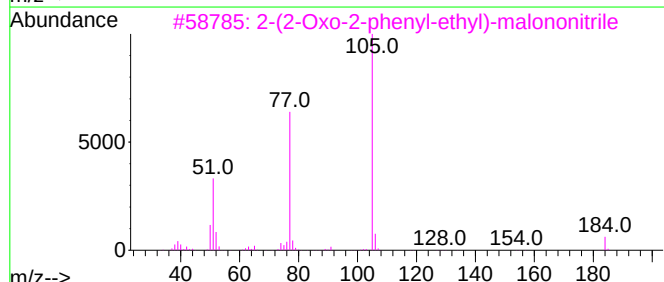
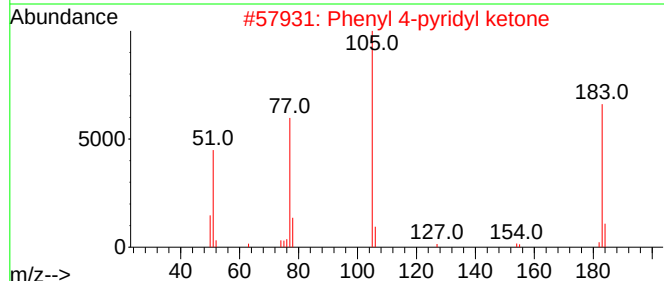
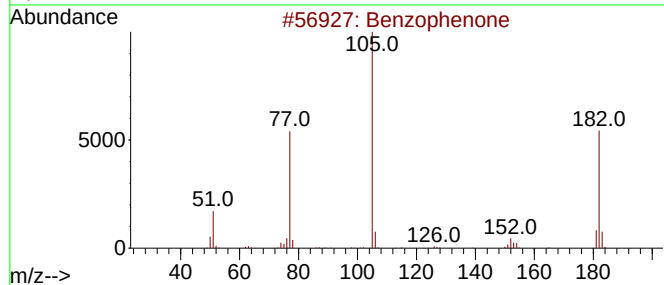
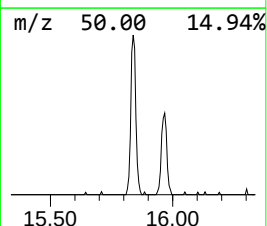
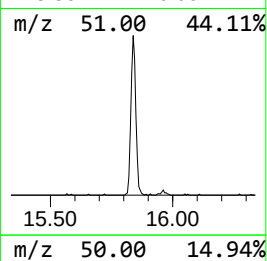
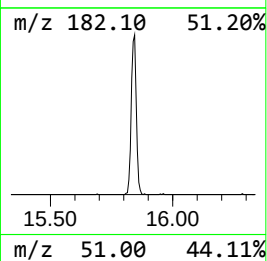
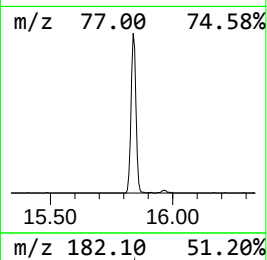
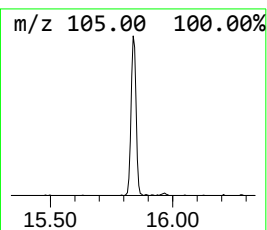
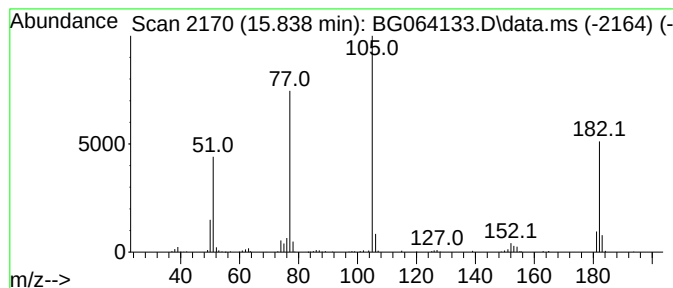
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.838	16.12 ng	362796	Acenaphthene-d10	14.481

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	64
3			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	62
4			Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
5			Benzoylformic acid	150	C8H6O3	000611-73-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040125\
Data File : BG064133.D
Acq On : 1 Apr 2025 13:43
Operator : RC/JU
Sample : Q1672-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-8

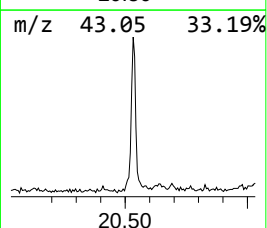
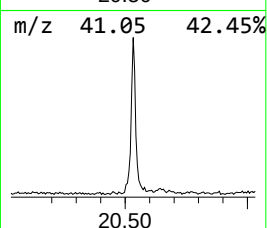
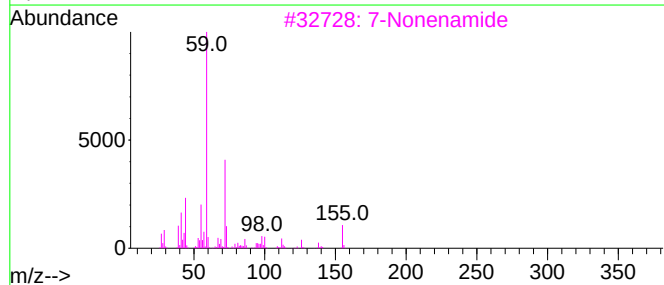
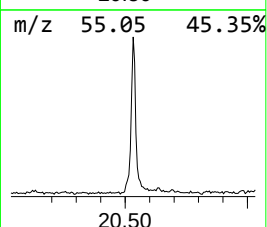
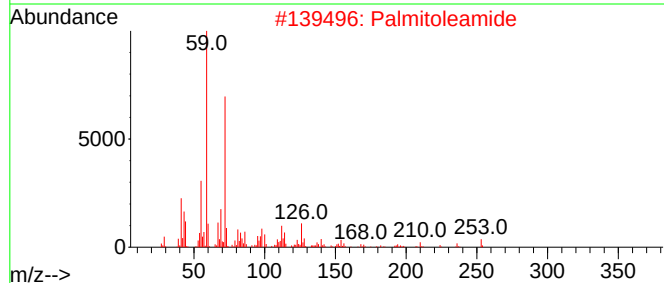
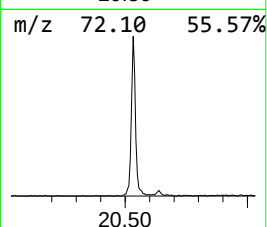
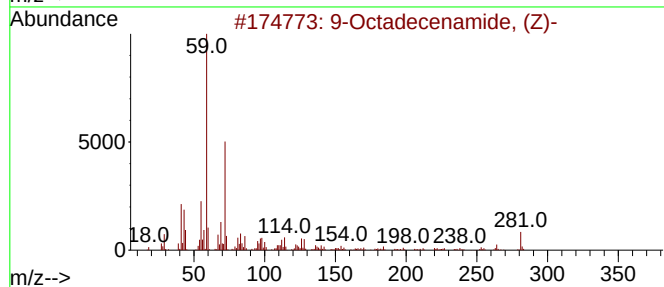
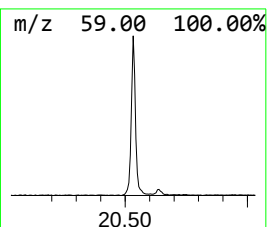
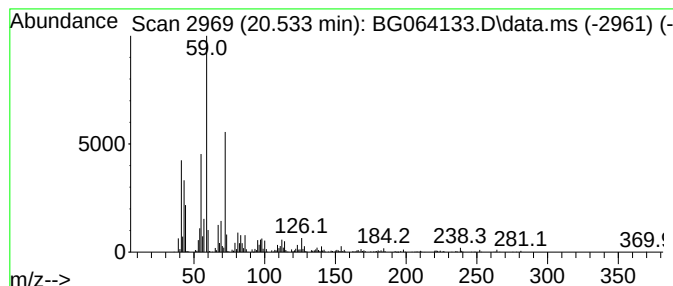
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.532	26.54 ng	918970	Chrysene-d12	21.449

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		Palmitoleamide	253	C16H31NO	106010-22-4	64
3		7-Nonenamide	155	C9H17NO	090949-53-4	59
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		Octanamide	143	C8H17NO	000629-01-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040125\
Data File : BG064133.D
Acq On : 1 Apr 2025 13:43
Operator : RC/JU
Sample : Q1672-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-8

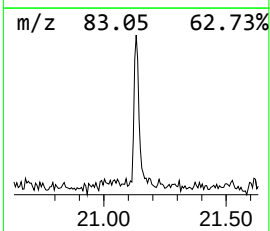
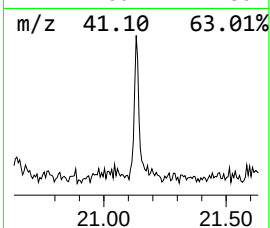
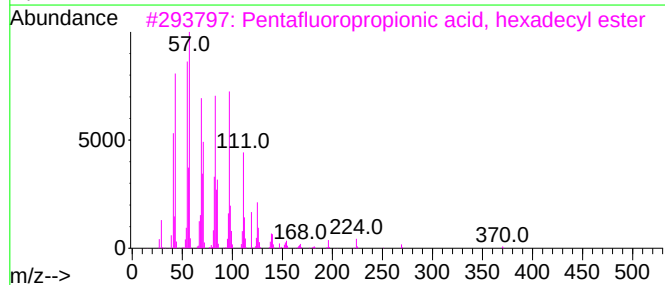
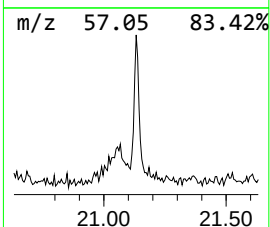
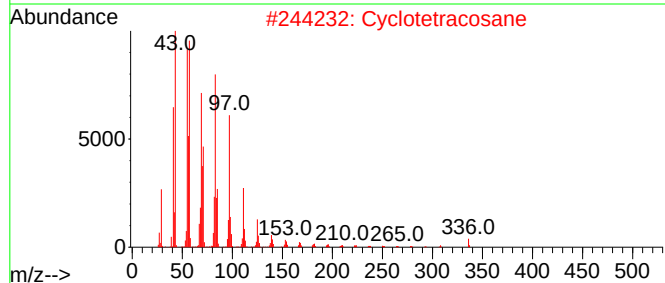
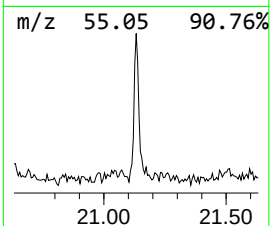
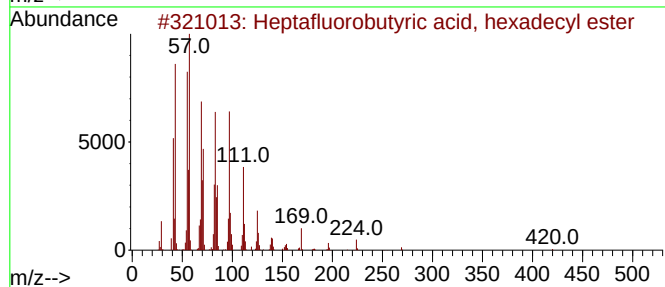
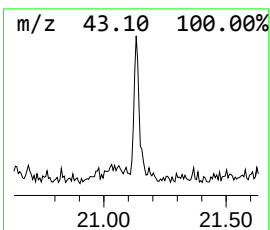
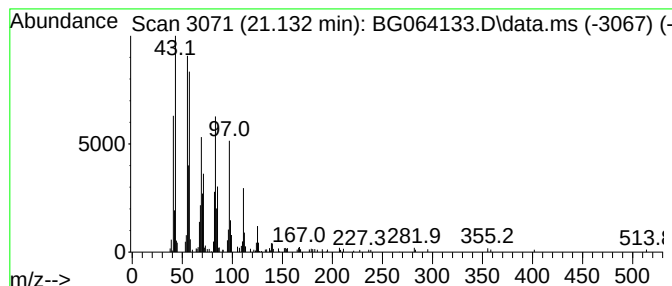
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.132	5.66 ng	196096	Chrysene-d12	21.449

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2			Cyclotetracosane	336	C24H48	000297-03-0	91
3			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040125\
Data File : BG064133.D
Acq On : 1 Apr 2025 13:43
Operator : RC/JU
Sample : Q1672-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-8

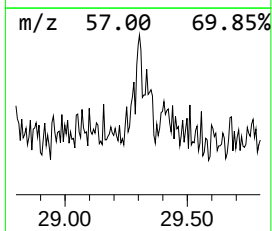
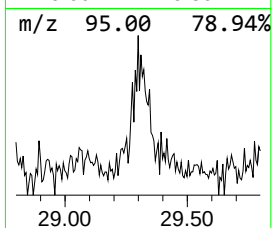
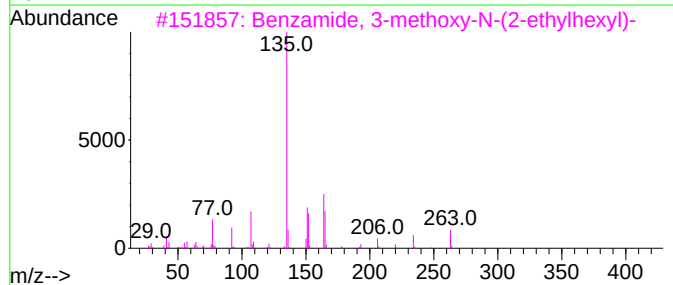
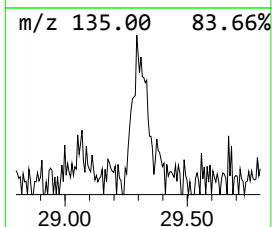
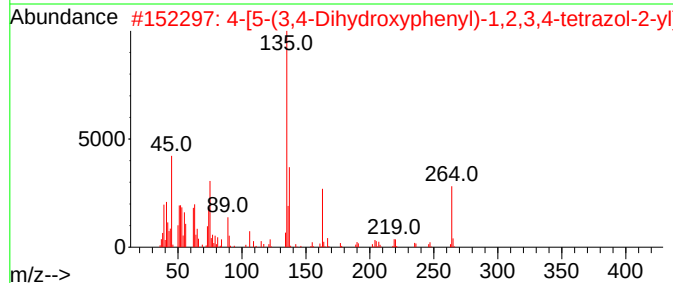
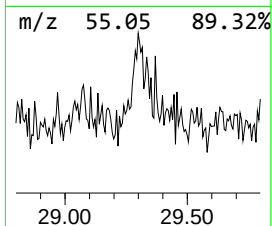
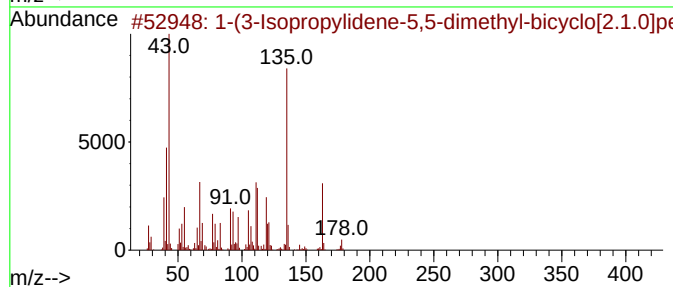
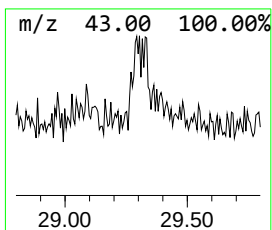
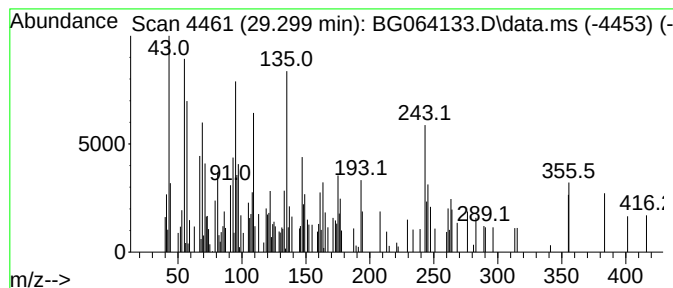
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown29.299 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.299	2.24 ng	79314	Perylene-d12	24.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(3-Isopropylidene-5,5-dimethyl...	178	C12H18O	1000185-69-1	25		
2	4-[5-(3,4-Dihydroxyphenyl)-1,2,3...	264	C11H12N4O4	1000410-76-1	18		
3	Benzamide, 3-methoxy-N-(2-ethylh...	263	C16H25NO2	1000407-51-4	14		
4	Benzo[1,3]dioxol-5-ylmethyl-(1-p...	261	C12H15N5O2	1000275-83-0	14		
5	Benzamide, N-(1-adamantyl)hydrox...	283	C18H21NO2	1000272-00-5	11		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040125\
Data File : BG064133.D
Acq On : 1 Apr 2025 13:43
Operator : RC/JU
Sample : Q1672-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.986	10.5	ng	121889	1	7.859	232574	20.0
Benzophenone	15.838	16.1	ng	362796	3	14.481	450191	20.0
9-Octadecenamid...	20.532	26.5	ng	918970	5	21.449	692581	20.0
Heptafluorobuty...	21.132	5.7	ng	196096	5	21.449	692581	20.0
unknown29.299	29.299	2.2	ng	79314	6	24.463	707782	20.0