

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010524\
 Data File : BG060269.D
 Acq On : 5 Jan 2024 13:56
 Operator : MA/JU
 Sample : 05964-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMA3

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-BG122923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.116	3	5	19	rVB	1662293	2319944	13.12%	3.429%
2	5.508	405	412	426	rVB	1738251	2788532	15.78%	4.121%
3	6.565	587	592	603	rVB2	155573	256403	1.45%	0.379%
4	7.094	674	682	698	rBV	1005562	1757922	9.95%	2.598%
5	7.934	817	825	830	rBV	750243	1278894	7.24%	1.890%
6	7.987	830	834	843	rVB	129709	211349	1.20%	0.312%
7	9.027	1005	1011	1015	rBV	145278	244634	1.38%	0.362%
8	9.092	1015	1022	1034	rVB	2396227	4289243	24.27%	6.339%
9	10.737	1293	1302	1309	rBV	963706	1737357	9.83%	2.568%
10	12.923	1669	1674	1682	rVB	139129	205362	1.16%	0.304%
11	13.193	1711	1720	1734	rBV	6481748	10568581	59.79%	15.620%
12	14.568	1946	1954	1963	rBV	1616891	2553906	14.45%	3.775%
13	16.060	2200	2208	2219	rBV	5172837	8096443	45.80%	11.966%
14	17.317	2416	2422	2435	rBV	2278455	3387131	19.16%	5.006%
15	17.981	2530	2535	2540	rBV	961375	1298329	7.35%	1.919%
16	19.938	2862	2868	2879	rBV	12154249	17676054	100.00%	26.125%
17	21.583	3142	3148	3157	rBV2	2662775	4263148	24.12%	6.301%
18	24.756	3678	3688	3703	rBV	1734640	4726504	26.74%	6.986%

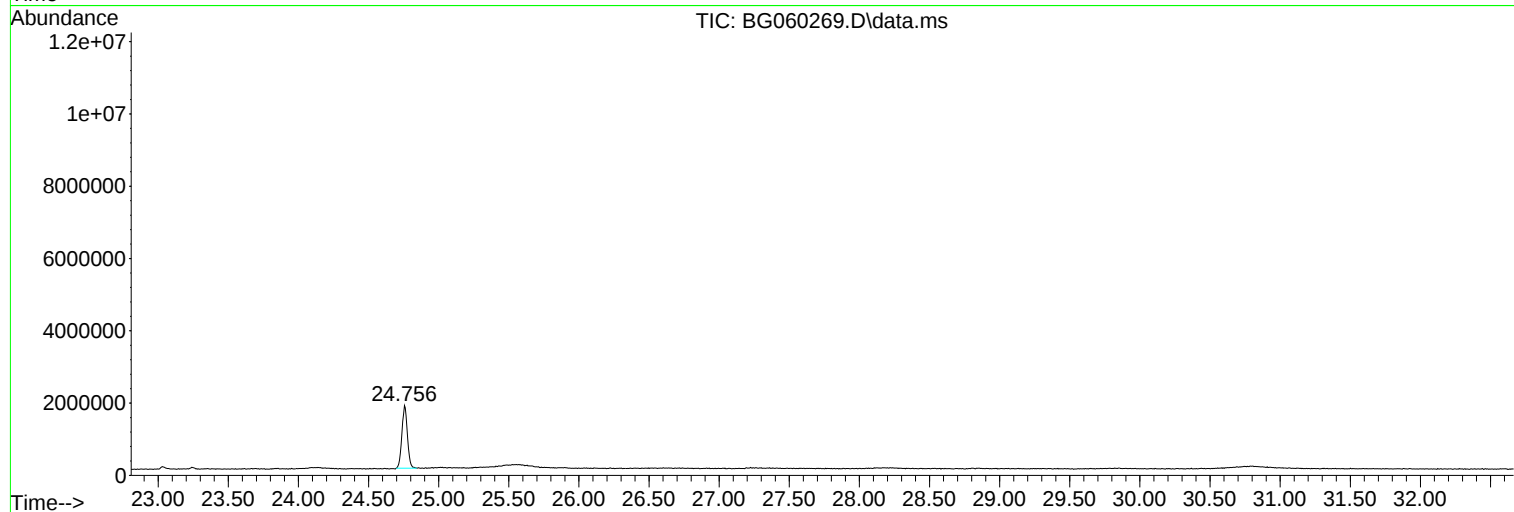
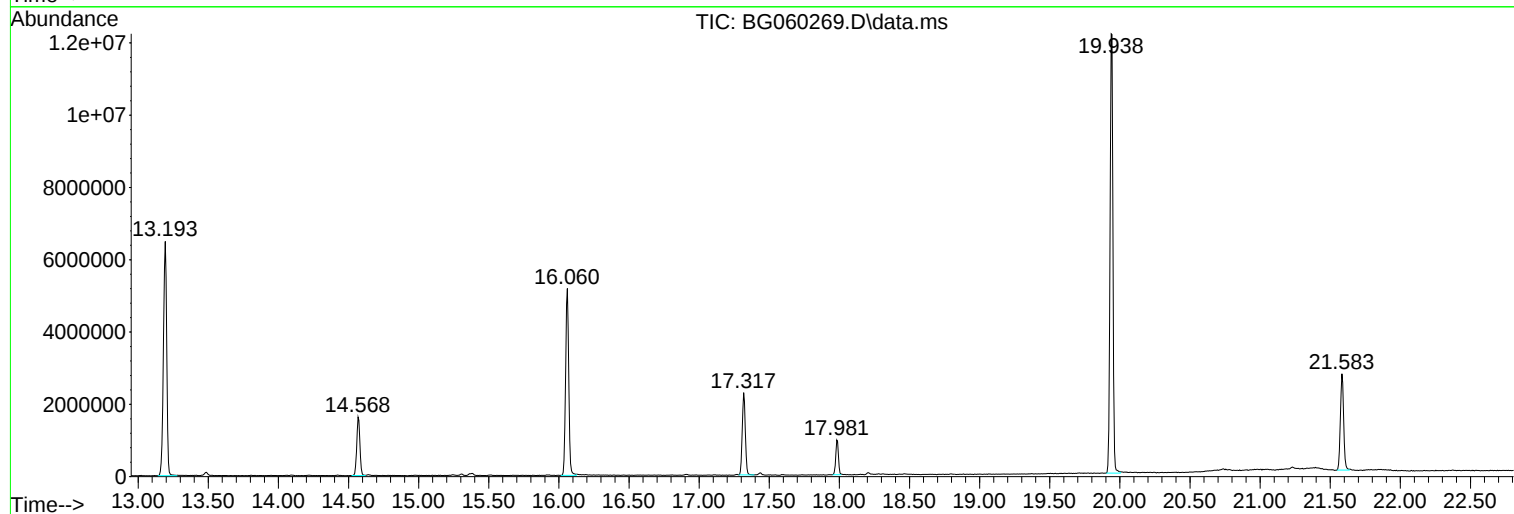
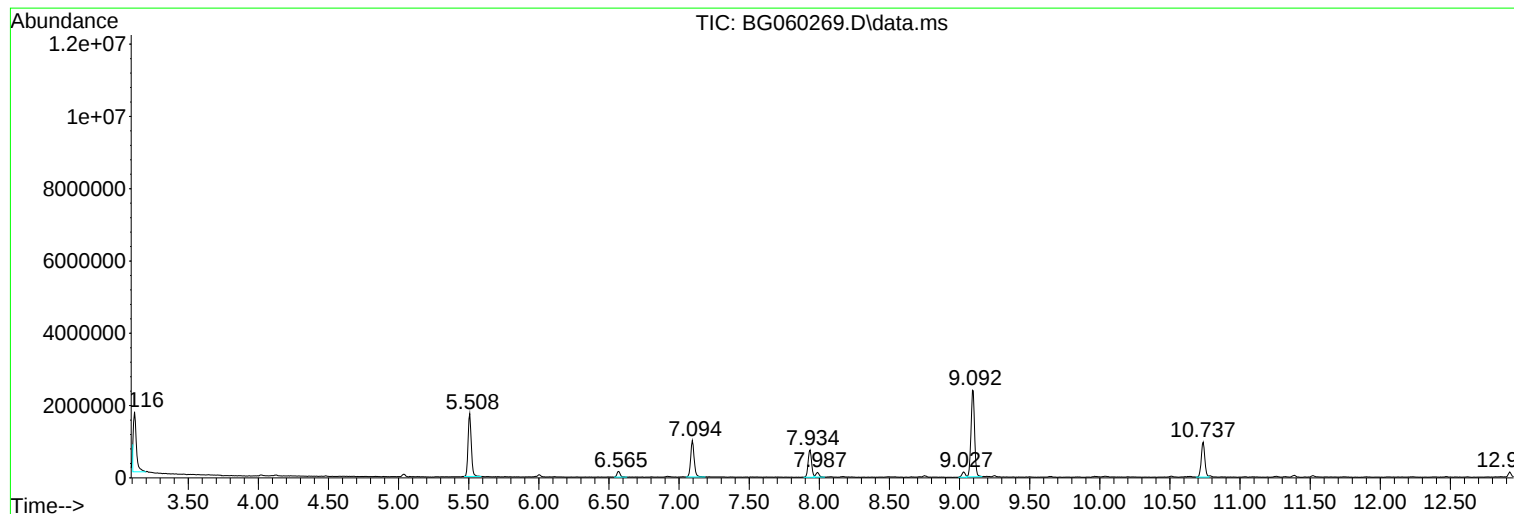
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG060269.D
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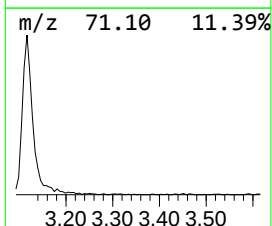
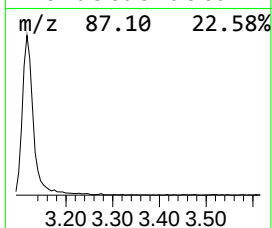
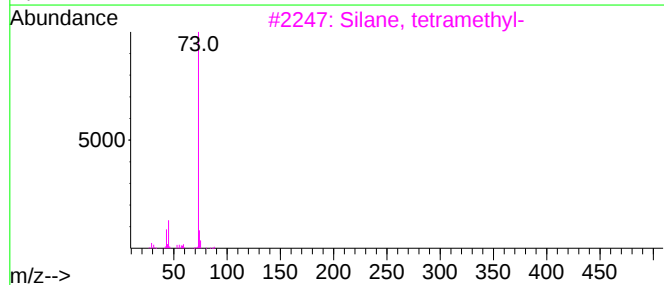
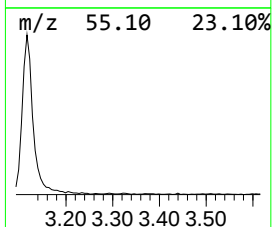
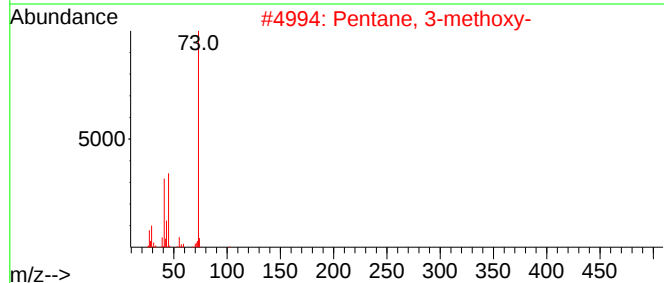
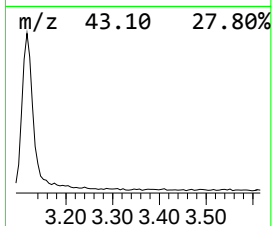
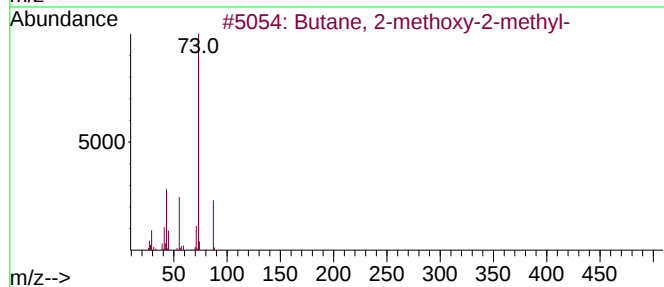
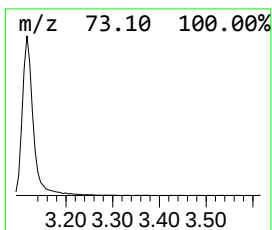
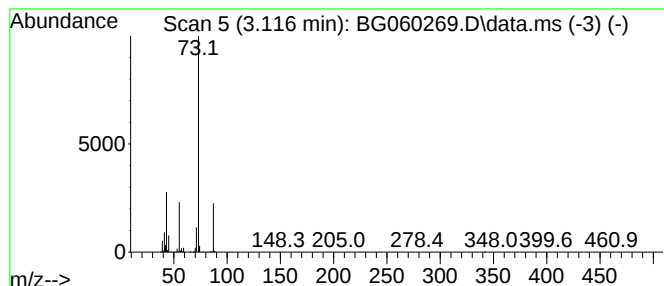
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.116	36.28 ng	2319940	1,4-Dichlorobenzene-d4	7.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9



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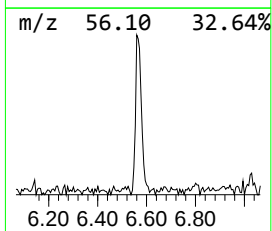
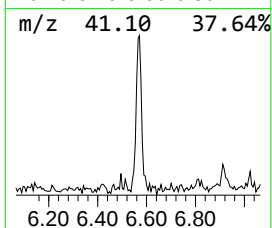
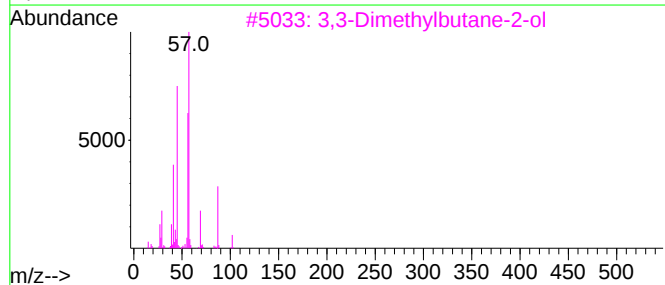
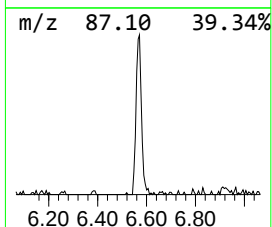
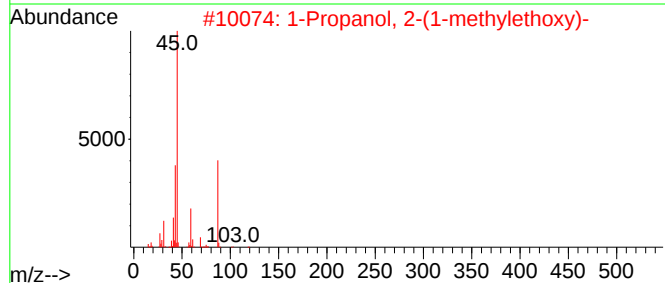
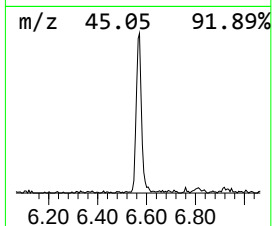
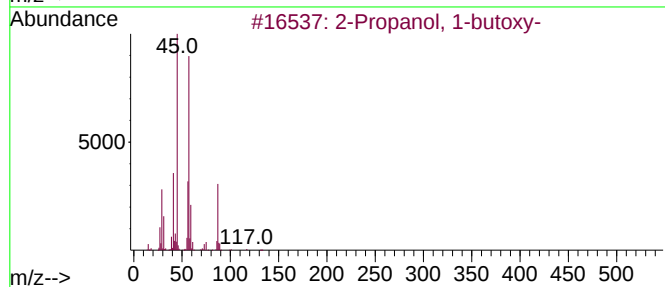
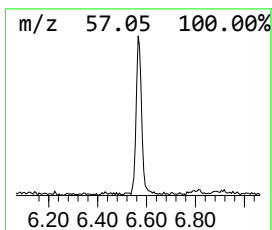
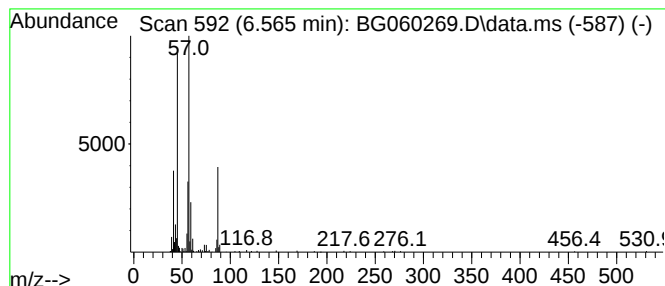
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Propanol, 1-butoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.565	4.01 ng	256403	1,4-Dichlorobenzene-d4	7.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	83
2			1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	53
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4			DL-Lactamide, N,O-dipropyl-	173	C9H19NO2	1010452-56-1	50
5			Propane, 1,1'-[ethylidenebis(oxy...]	146	C8H18O2	000105-82-8	47



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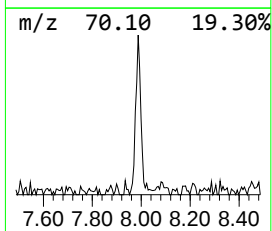
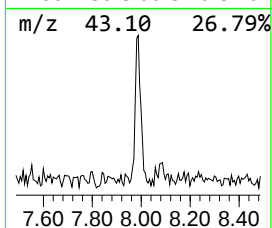
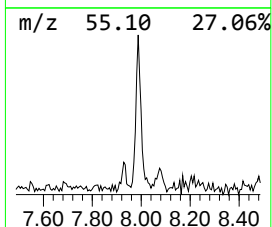
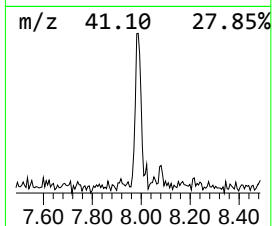
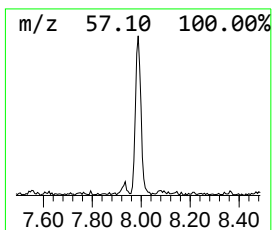
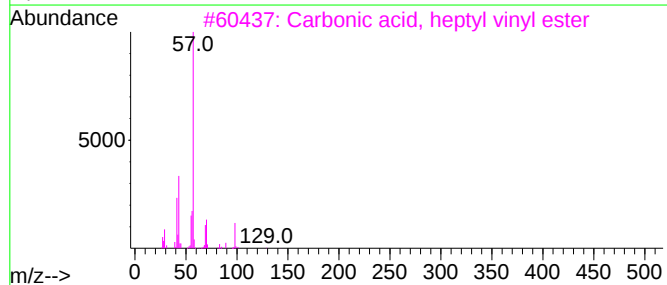
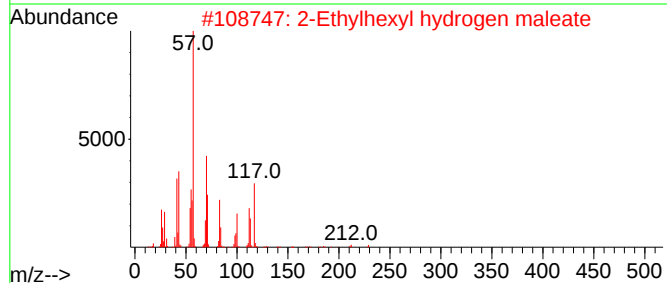
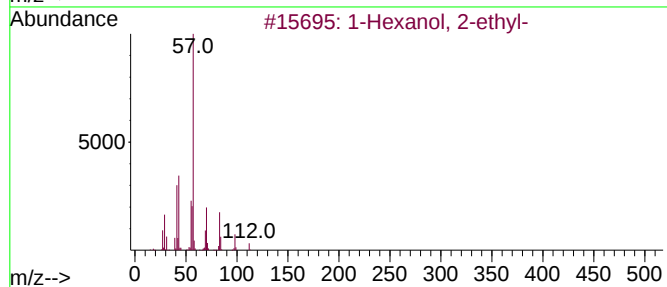
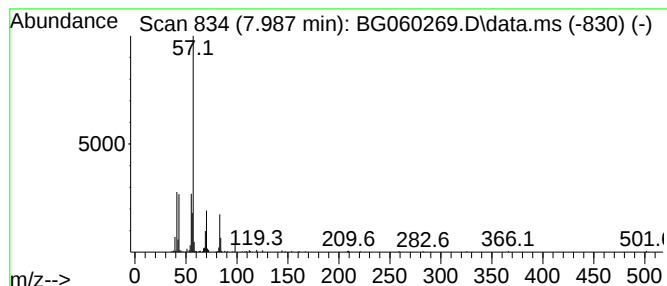
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.987	3.31 ng	211349	1,4-Dichlorobenzene-d4	7.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			2-Ethylhexyl hydrogen maleate	228	C12H20O4	002370-71-0	50
3			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	50
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	45
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	43



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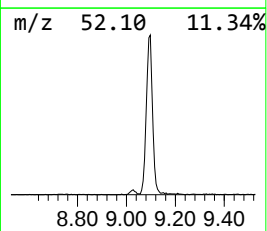
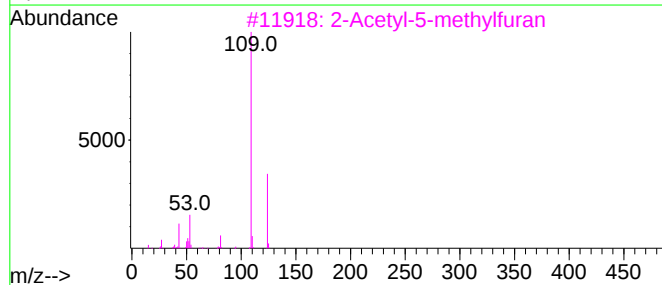
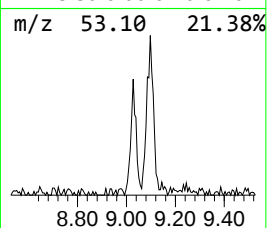
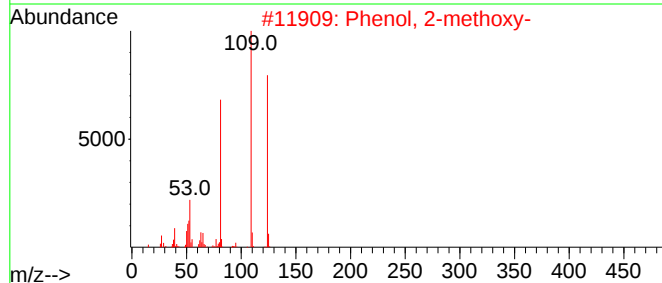
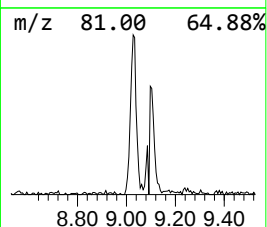
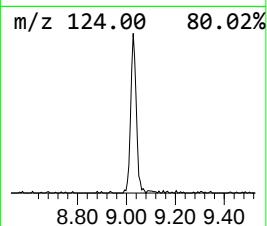
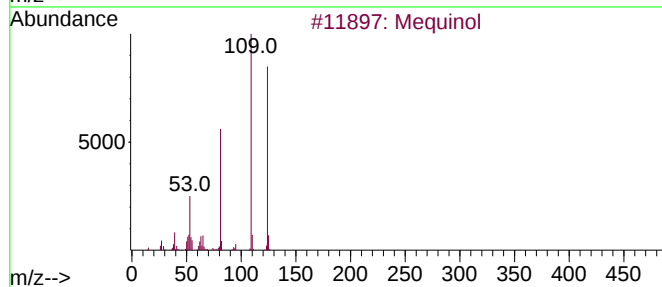
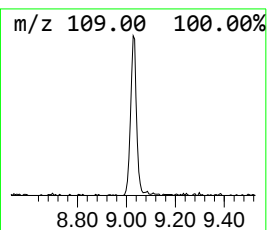
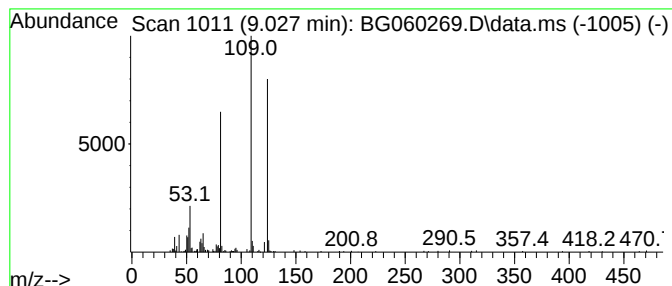
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Mequinol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.027	3.83 ng	244634	1,4-Dichlorobenzene-d4	7.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mequinol	124	C7H8O2	000150-76-5	90
2			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	87
3			2-Acetyl-5-methylfuran	124	C7H8O2	001193-79-9	86
4			3-Fluoro-o-xylene	124	C8H9F	000443-82-3	64
5			5-Ethyl-2-furaldehyde	124	C7H8O2	023074-10-4	58



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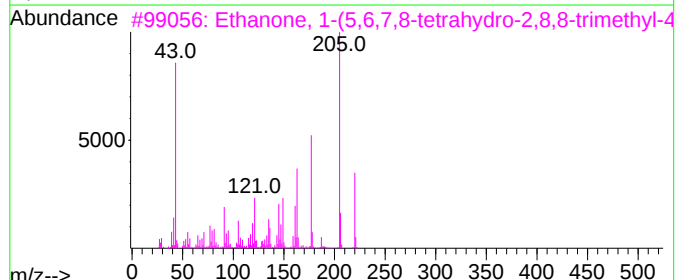
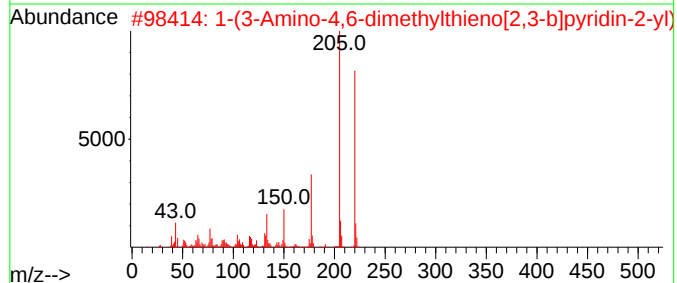
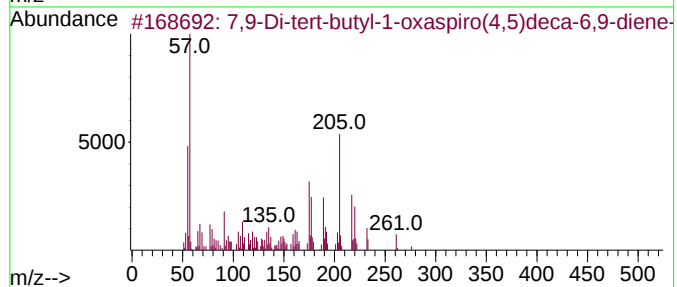
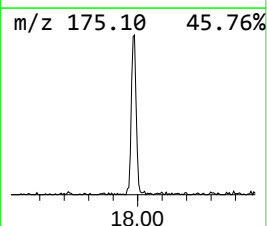
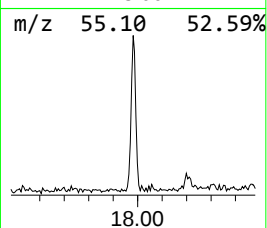
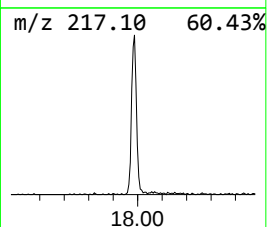
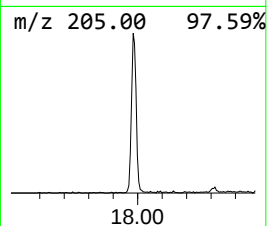
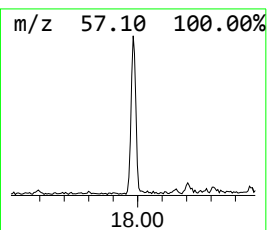
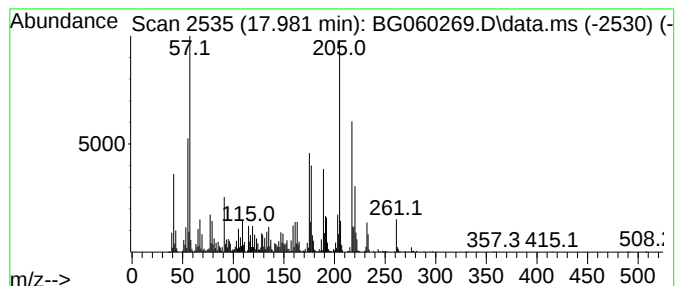
Instrument :
BNA_G
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.981	7.67 ng	1298330	Phenanthrene-d10	17.317	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	97
2	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	43
3	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	43
4	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	42
5	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	38



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.116	36.3	ng	2319940	1	7.934	1278890	20.0
2-Propanol, 1-b...	6.565	4.0	ng	256403	1	7.934	1278890	20.0
1-Hexanol, 2-et...	7.987	3.3	ng	211349	1	7.934	1278890	20.0
Mequinol	9.027	3.8	ng	244634	1	7.934	1278890	20.0
7,9-Di-tert-but...	17.981	7.7	ng	1298330	4	17.317	3387130	20.0