

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062622\
 Data File : BG054081.D
 Acq On : 26 Jun 2022 20:32
 Operator : CG/JU
 Sample : N3488-14
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-13-15-17-20220623

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-BG061322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054081.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.640	375	383	396	rBV	504168	865730	30.84%	7.338%
2	7.233	646	654	664	rBV	511688	920652	32.80%	7.803%
3	8.073	789	797	802	rBV	90399	160241	5.71%	1.358%
4	8.132	802	807	816	rVB	22410	38892	1.39%	0.330%
5	9.230	986	994	1007	rBV	318314	593904	21.16%	5.034%
6	10.876	1266	1274	1283	rVB	120406	229303	8.17%	1.943%
7	13.320	1683	1690	1698	rBV	916762	1441299	51.35%	12.216%
8	13.907	1784	1790	1807	rBV	156248	252958	9.01%	2.144%
9	14.695	1916	1924	1934	rBV	206672	329923	11.75%	2.796%
10	16.181	2170	2177	2192	rBV	707077	1125776	40.11%	9.542%
11	17.438	2383	2391	2398	rBV	284746	459253	16.36%	3.892%
12	18.326	2536	2542	2551	rBV3	16653	30849	1.10%	0.261%
13	19.360	2713	2718	2728	rBV	47490	66992	2.39%	0.568%
14	20.047	2828	2835	2842	rBV	2086415	2806996	100.00%	23.791%
15	20.729	2943	2951	2965	rBV	869777	1213870	43.24%	10.288%
16	21.357	3053	3058	3069	rVB2	24093	44208	1.57%	0.375%
17	21.710	3111	3118	3128	rBV2	346112	590377	21.03%	5.004%
18	22.239	3203	3208	3213	rBV	23187	35616	1.27%	0.302%
19	24.965	3661	3672	3687	rVB2	208620	591799	21.08%	5.016%

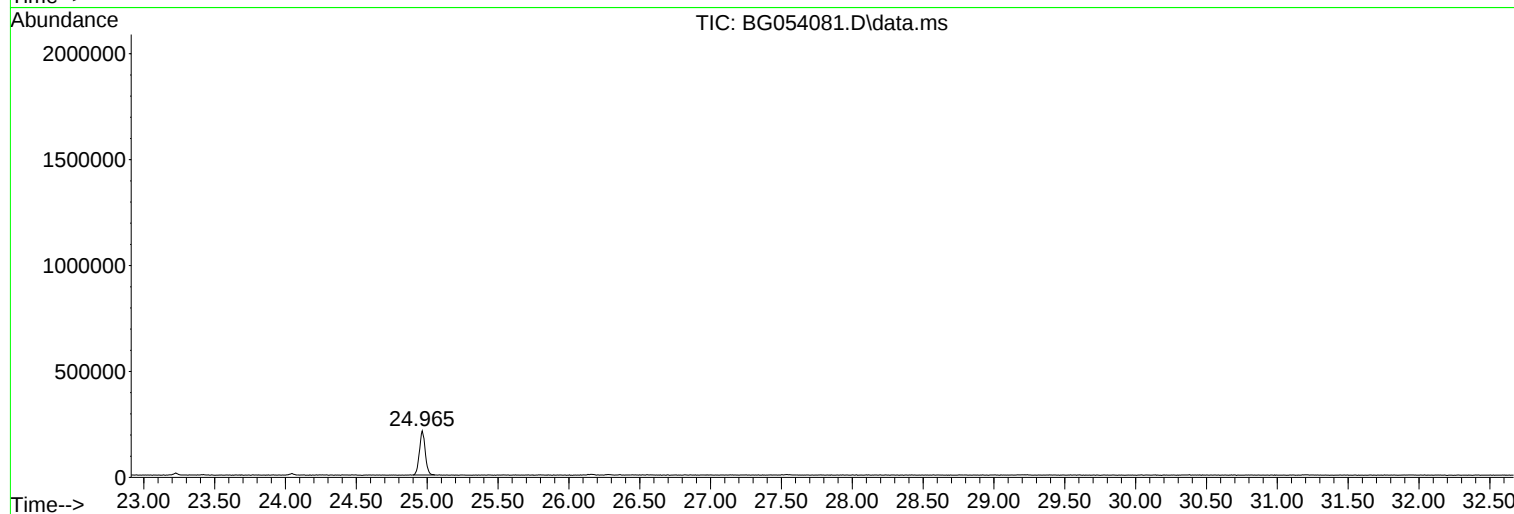
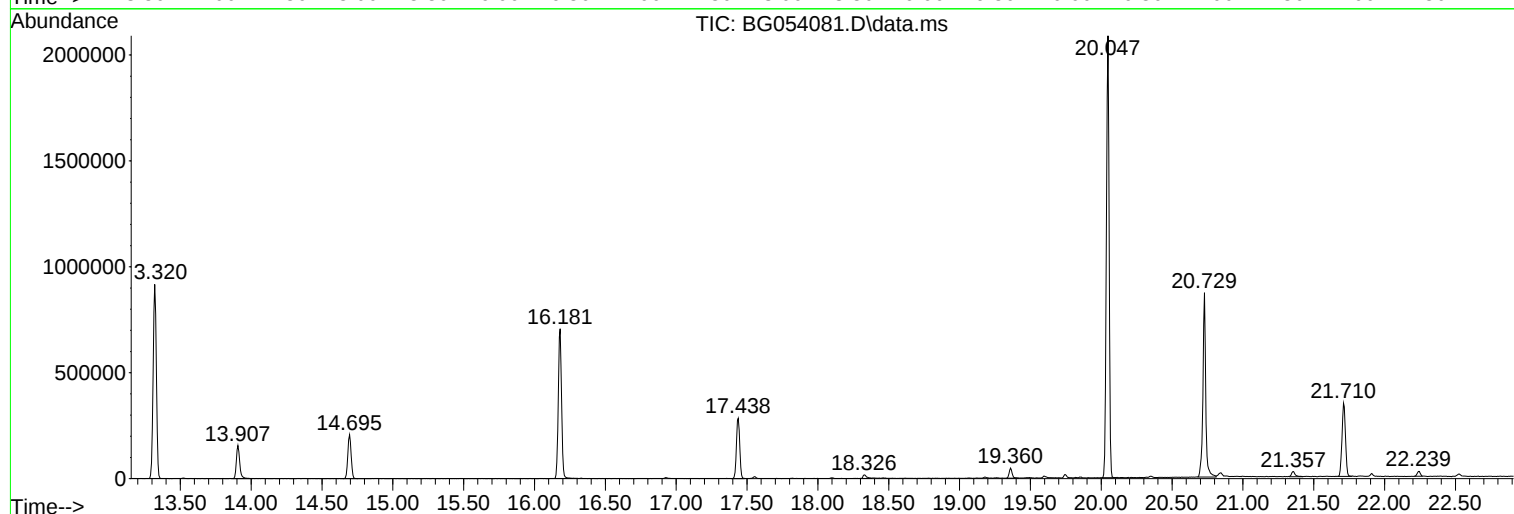
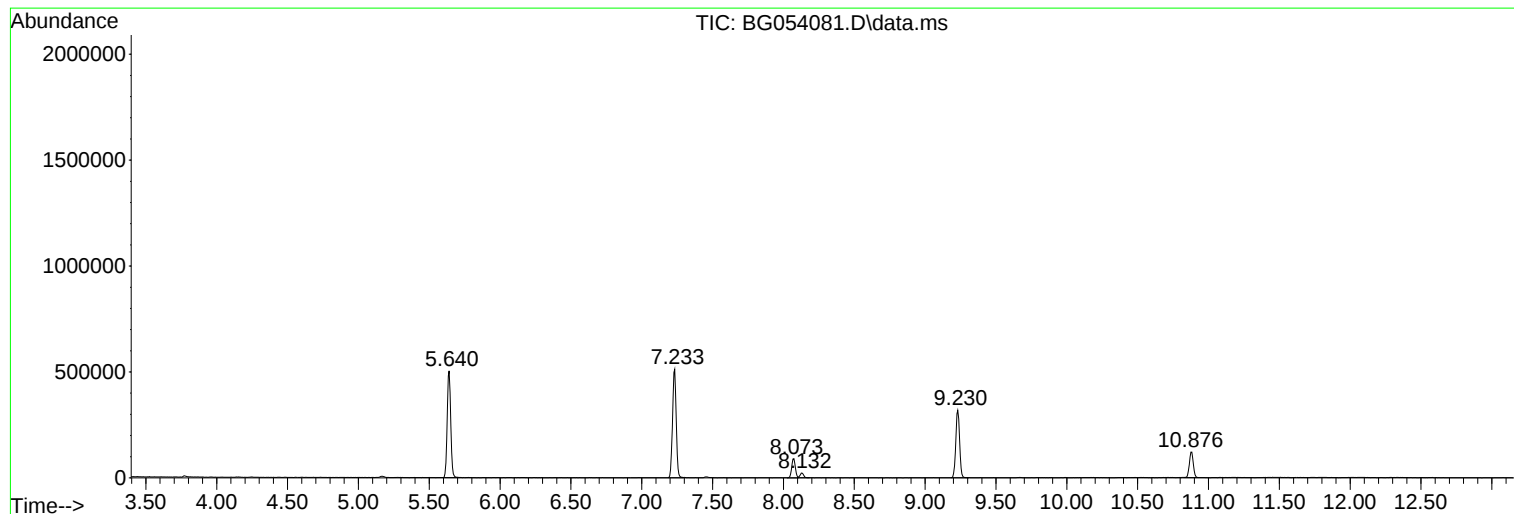
Sum of corrected areas: 11798638

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.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 : BG054081.D
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BNA_G
ClientSampleId :
SB-13-15-17-20220623

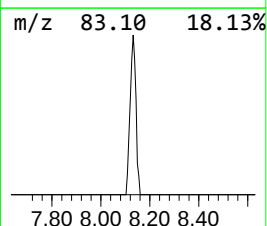
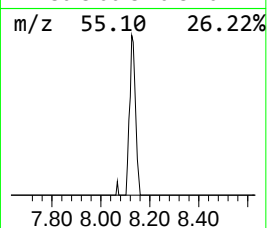
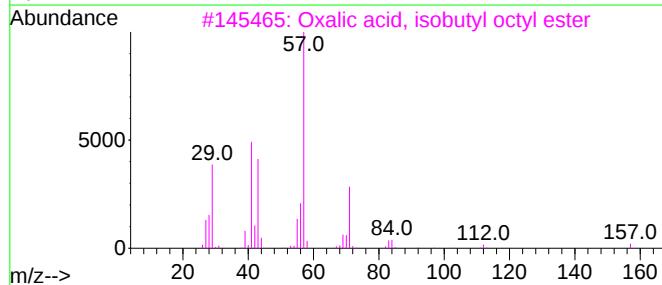
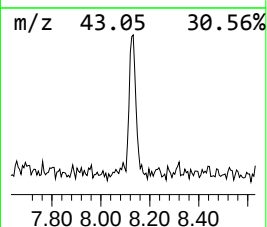
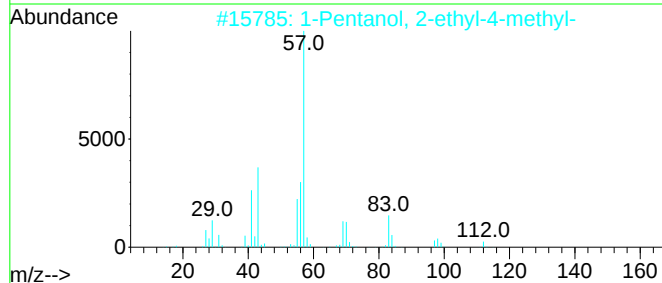
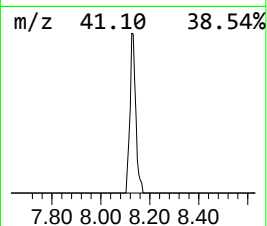
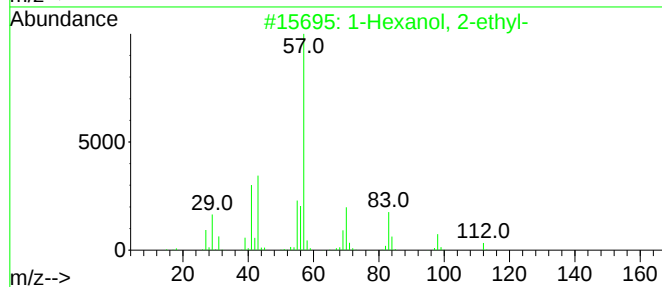
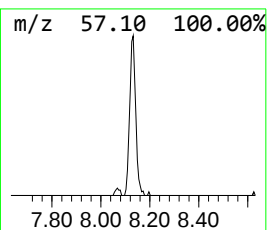
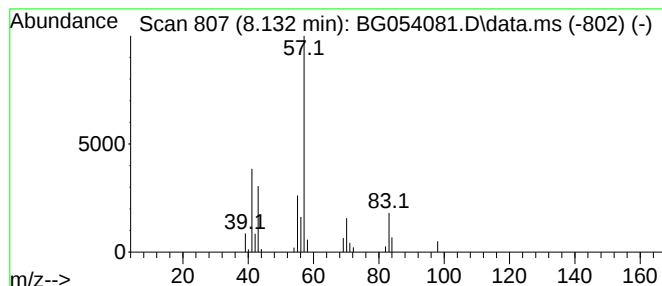
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.132	4.85 ng	38892	1,4-Dichlorobenzene-d4	8.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	42
3			Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	40
4			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	40
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	40



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ALS Vial : 11 Sample Multiplier: 1

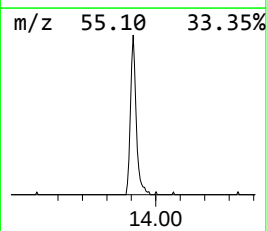
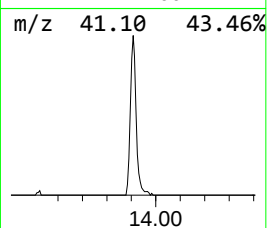
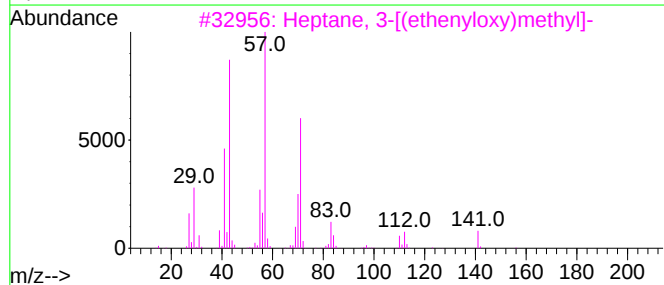
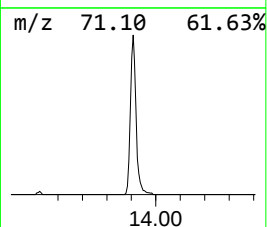
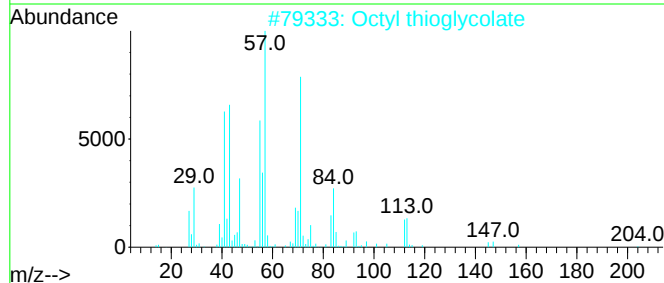
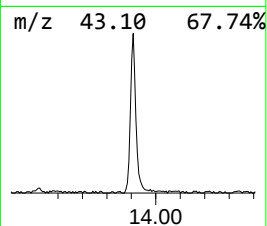
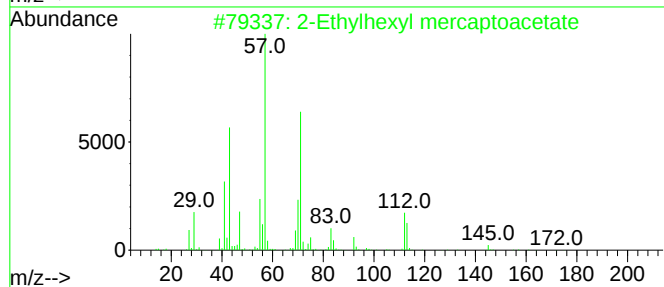
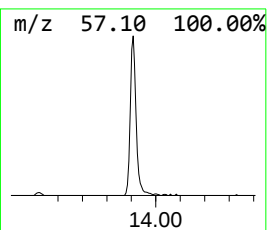
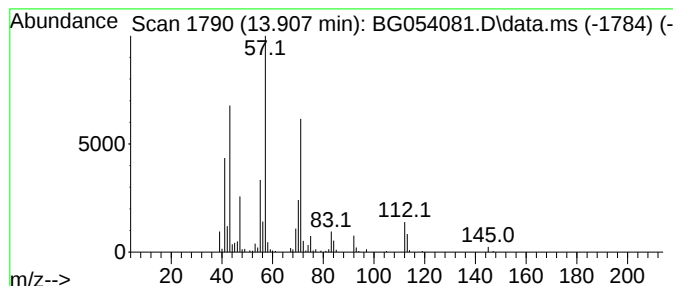
Instrument :
BNA_G
ClientSampleId :
SB-13-15-17-20220623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.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-Ethylhexyl mercaptoacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.907	15.33 ng	252958	Acenaphthene-d10		14.695	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Ethylhexyl mercaptoacetate		204	C10H20O2S	007659-86-1	72
2	Octyl thioglycolate		204	C10H20O2S	007664-80-4	64
3	Heptane, 3-[(ethenyloxy)methyl]-		156	C10H20O	000103-44-6	53
4	Oxalic acid, 2-ethylhexyl hexyl ...		286	C16H30O4	1000309-38-9	53
5	Decane, 5,6-dipropyl-		226	C16H34	119209-20-0	50



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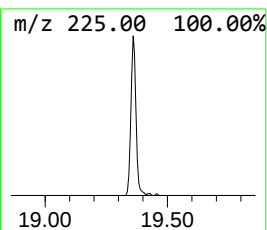
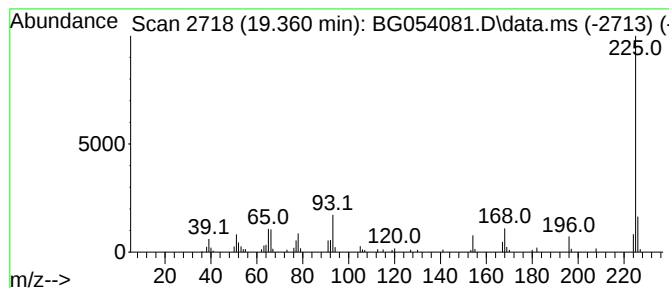
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

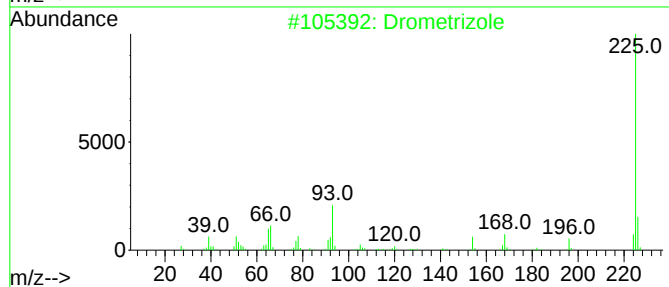
Peak Number 3 Drometrizole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.360	2.92 ng	66992	Phenanthrene-d10	17.438

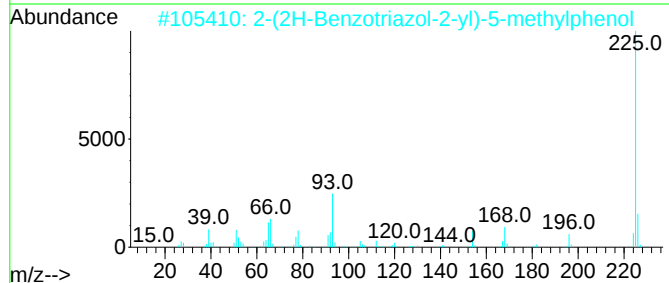
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Drometrizole	225	C13H11N3O	002440-22-4	97
2			2-(2H-Benzotriazol-2-yl)-5-methy...	225	C13H11N3O	004998-48-5	96
3			9(10H)-Acridinone, 1-hydroxy-10-...	225	C14H11NO2	016584-54-6	80
4			Propionitrile, 3-(5-methyl-3-phe...	225	C13H11N3O	1000263-77-0	80
5			4-Amino-2-oxo-1,2-dihydro[1]benz...	225	C12H7N3O2	078993-57-4	59



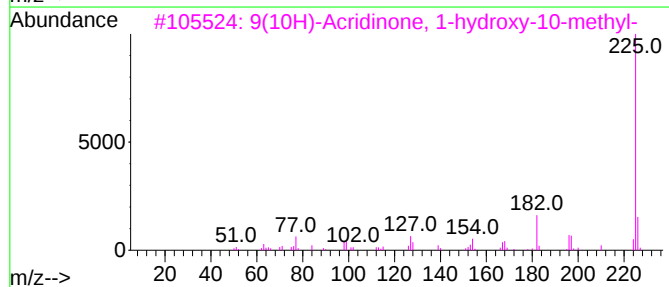
m/z 93.10 17.23%



m/z 226.00 16.44%



m/z 168.00 10.97%



m/z 65.00 10.76%

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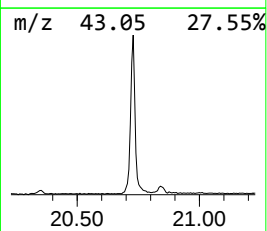
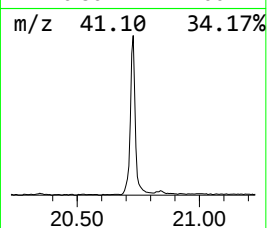
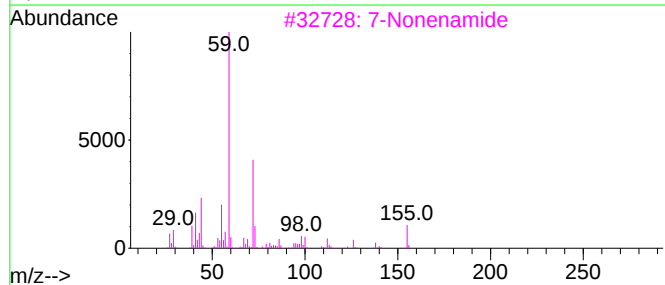
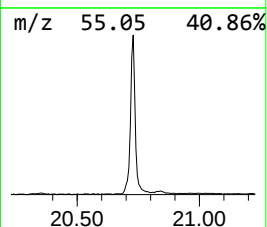
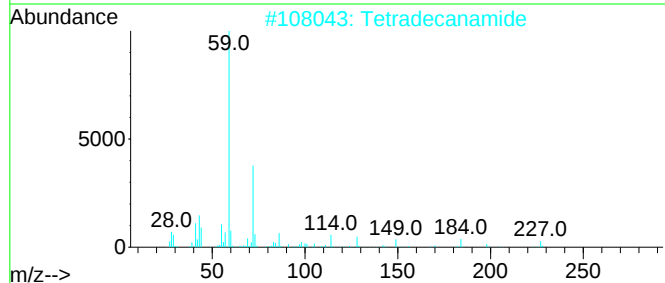
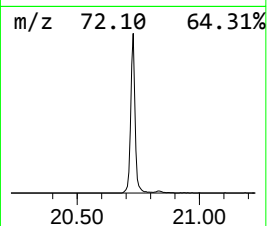
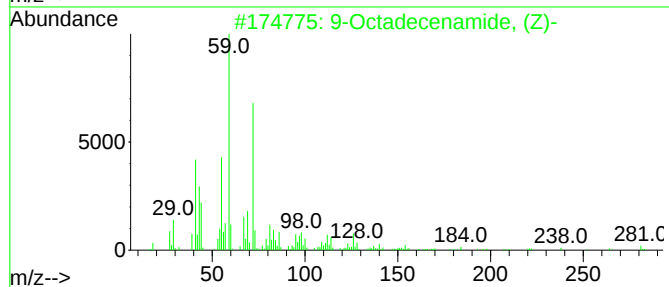
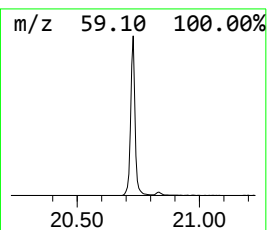
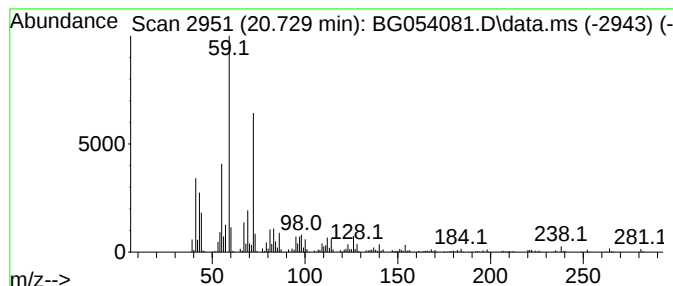
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.729	41.12 ng	1213870	Chrysene-d12	21.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-			281	C18H35NO	000301-02-0	99
2	Tetradecanamide			227	C14H29NO	000638-58-4	72
3	7-Nonenamide			155	C9H17NO	090949-53-4	64
4	Dodecanamide			199	C12H25NO	001120-16-7	59
5	Octanamide			143	C8H17NO	000629-01-6	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	8.132	4.8	ng	38892	1	8.073	160241	20.0
2-Ethylhexyl me...	13.907	15.3	ng	252958	3	14.695	329923	20.0
Drometrizole	19.360	2.9	ng	66992	4	17.438	459253	20.0
9-Octadecenamid...	20.729	41.1	ng	1213870	5	21.710	590377	20.0