

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
 Data File : BG059885.D
 Acq On : 25 Nov 2023 10:35
 Operator : MA/JU
 Sample : 05366-01
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P-13(10-15)

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-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059885.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.809	405	412	420	rBV	348259	558468	36.40%	6.651%
2	7.436	683	689	697	rBV3	326182	569698	37.13%	6.785%
3	8.312	833	838	845	rBV2	102092	180421	11.76%	2.149%
4	9.516	1036	1043	1051	rVB	266995	469154	30.58%	5.588%
5	11.167	1315	1324	1329	rBV	165862	312183	20.35%	3.718%
6	11.214	1329	1332	1336	rVB2	19065	28418	1.85%	0.338%
7	13.018	1633	1639	1643	rVB4	10007	19767	1.29%	0.235%
8	13.570	1726	1733	1739	rBV	733357	1127036	73.45%	13.423%
9	13.770	1762	1767	1772	rBV4	9721	18930	1.23%	0.225%
10	14.323	1856	1861	1866	rVB3	8711	20731	1.35%	0.247%
11	14.622	1907	1912	1918	rBV3	62053	83376	5.43%	0.993%
12	14.910	1952	1961	1962	rBV3	21394	31967	2.08%	0.381%
13	14.945	1962	1967	1974	rVV	268132	425113	27.71%	5.063%
14	15.016	1974	1979	1983	rVB2	12969	18209	1.19%	0.217%
15	15.979	2139	2143	2151	rBV4	9521	20730	1.35%	0.247%
16	16.432	2213	2220	2226	rBV2	560235	832173	54.23%	9.911%
17	16.573	2237	2244	2247	rBV5	12690	21395	1.39%	0.255%
18	17.401	2381	2385	2391	rVB6	22821	26768	1.74%	0.319%
19	17.695	2429	2435	2440	rBV	291041	459706	29.96%	5.475%
20	17.742	2440	2443	2449	rVB2	58459	78080	5.09%	0.930%
21	18.512	2570	2574	2578	rBV7	34529	51173	3.34%	0.609%
22	18.612	2585	2591	2594	rVB7	16607	26033	1.70%	0.310%
23	18.747	2610	2614	2616	rBV3	15660	21206	1.38%	0.253%
24	19.041	2659	2664	2670	rBV10	13296	28674	1.87%	0.342%
25	19.458	2730	2735	2741	rBV7	27187	47215	3.08%	0.562%
26	19.734	2775	2782	2785	rBV	36459	60142	3.92%	0.716%
27	19.769	2785	2788	2791	rVB5	24713	28130	1.83%	0.335%
28	19.981	2821	2824	2828	rVB6	14734	18913	1.23%	0.225%
29	20.092	2840	2843	2850	rVB	44750	63690	4.15%	0.759%
30	20.274	2868	2874	2879	rVB	1155231	1534387	100.00%	18.274%
31	20.674	2937	2942	2945	rBV6	15946	24914	1.62%	0.297%
32	21.085	3009	3012	3014	rBV4	12844	17015	1.11%	0.203%
33	21.555	3088	3092	3098	rVB8	34563	61417	4.00%	0.731%
34	22.019	3163	3171	3178	rBV2	231424	461894	30.10%	5.501%
35	22.066	3178	3179	3185	rVB5	18912	25216	1.64%	0.300%
36	23.565	3426	3434	3440	rBV10	43392	99950	6.51%	1.190%

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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-BG111623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	24.428	3576	3581	3583	rBV6	13678	16725	1.09%	0.199%
38	25.398	3743	3746	3749	rBV5	12220	16069	1.05%	0.191%
39	25.580	3767	3777	3790	rBV	137430	440032	28.68%	5.241%
40	25.791	3811	3813	3818	rVB6	12441	19846	1.29%	0.236%
41	27.413	4085	4089	4093	rBV7	7749	15813	1.03%	0.188%
42	30.057	4536	4539	4546	rBV9	9160	15691	1.02%	0.187%

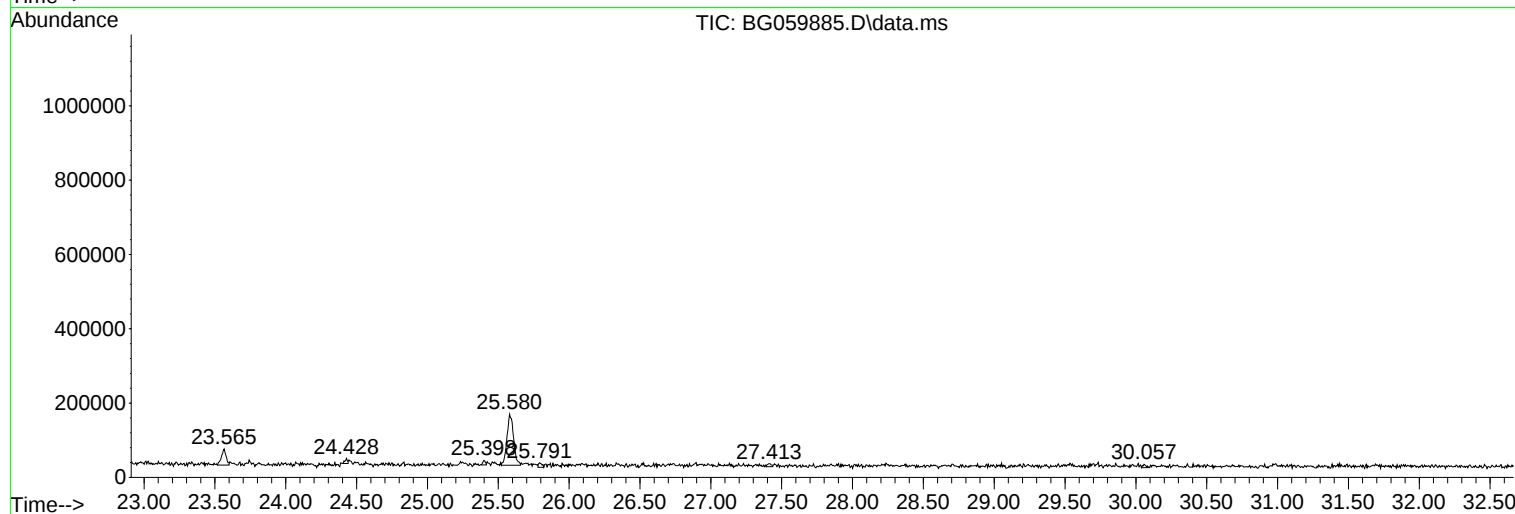
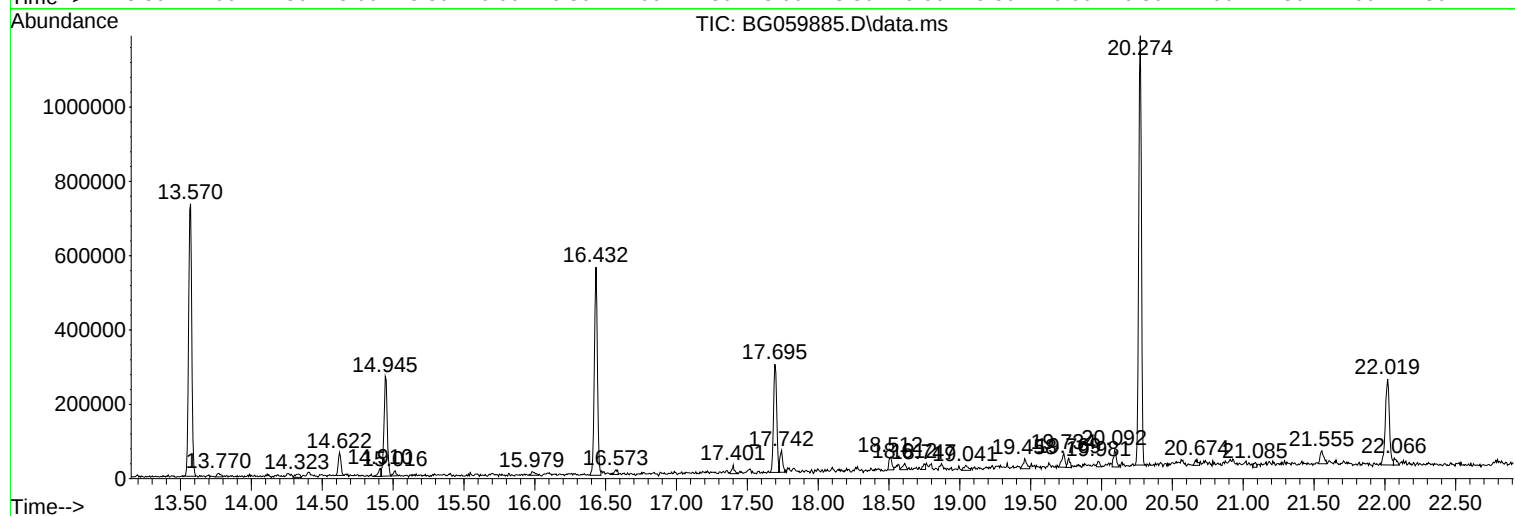
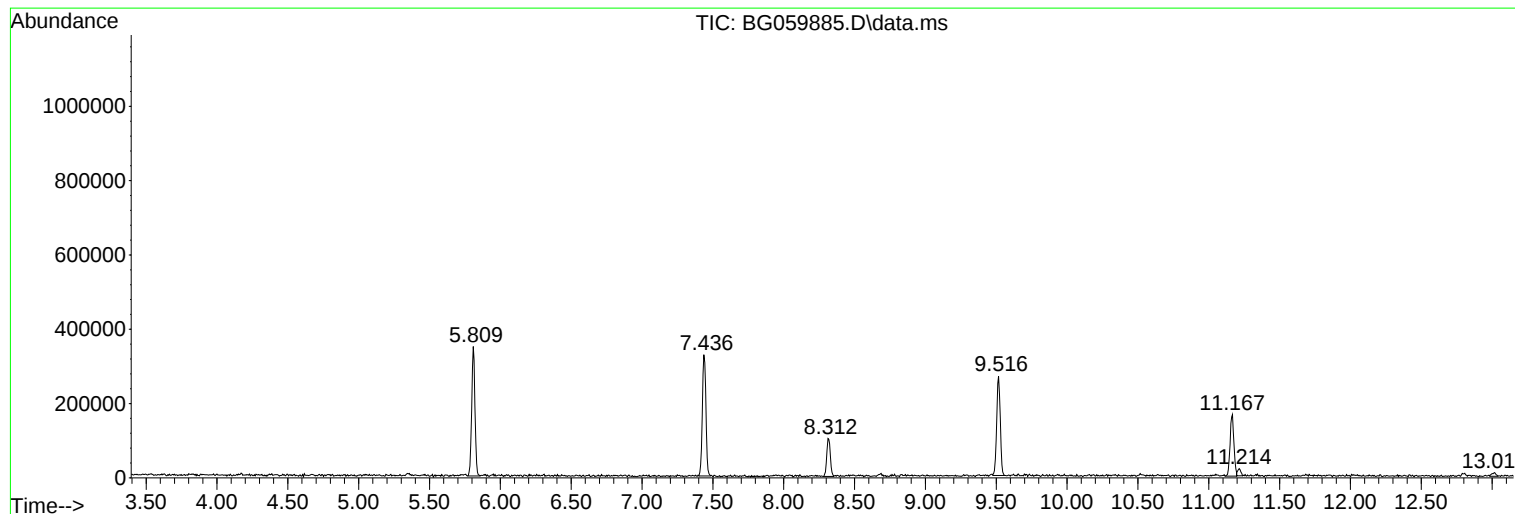
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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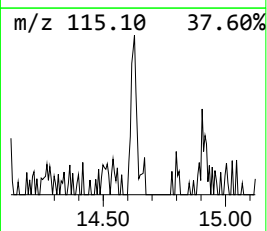
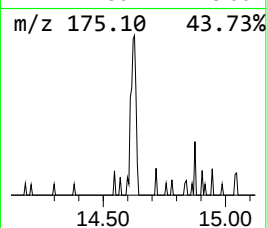
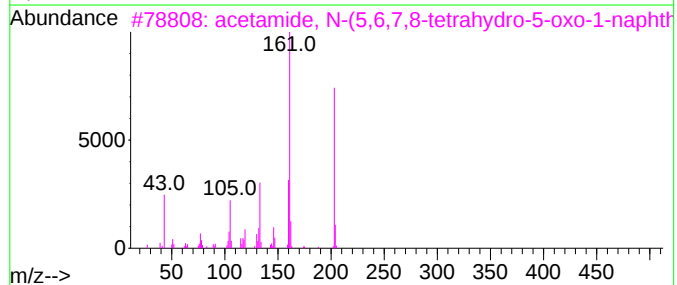
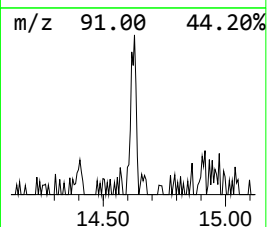
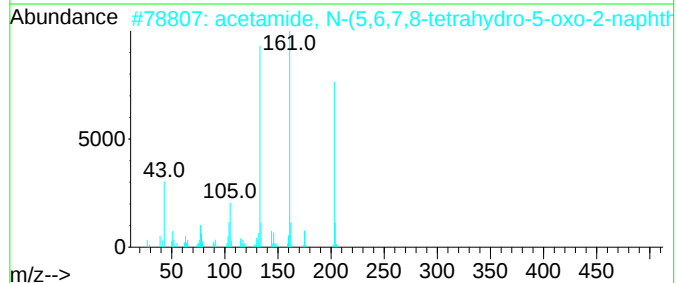
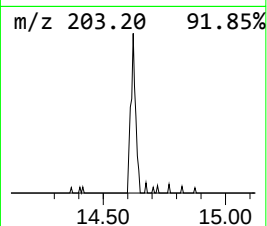
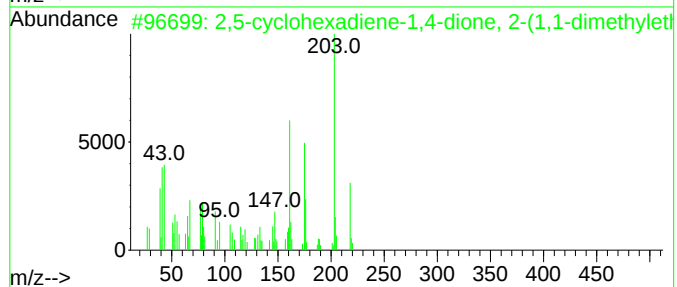
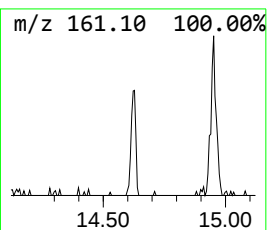
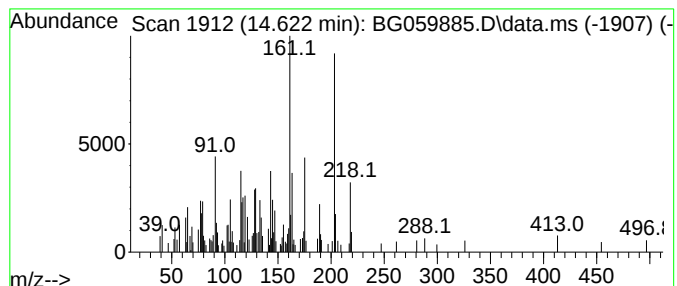
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,5-cyclohexadiene-1,4-dione... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.622	3.92 ng	83376	Acenaphthene-d10	14.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-cyclohexadiene-1,4-dione, 2-...	218	C14H18O2	1010396-22-4	64
2			acetamide, N-(5,6,7,8-tetrahydro...	203	C12H13NO2	1010400-45-2	49
3			acetamide, N-(5,6,7,8-tetrahydro...	203	C12H13NO2	1000400-45-4	46
4			2H-2,4a-Methanonaphthalene, 1,3,...	204	C15H24	001135-66-6	45
5			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	42



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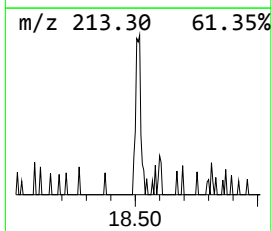
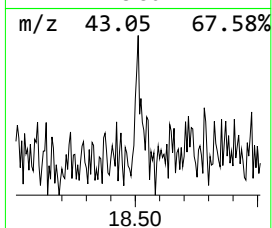
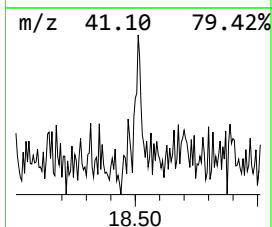
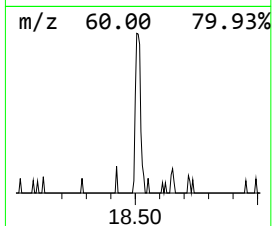
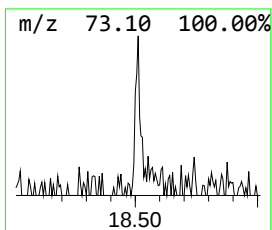
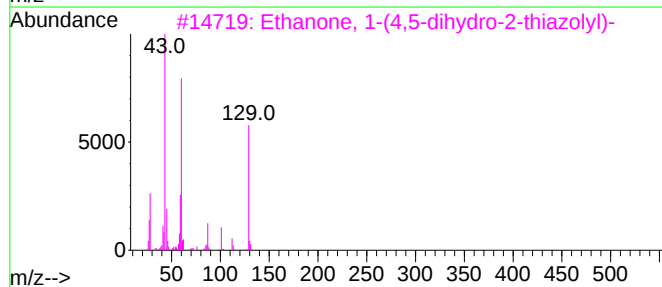
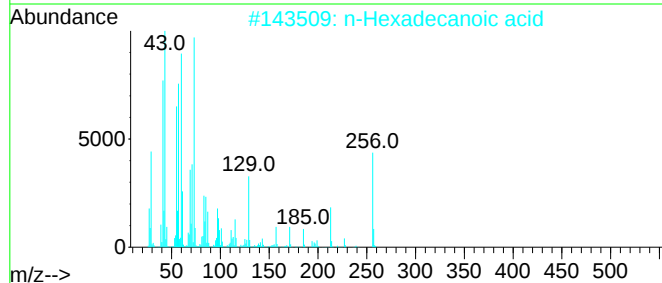
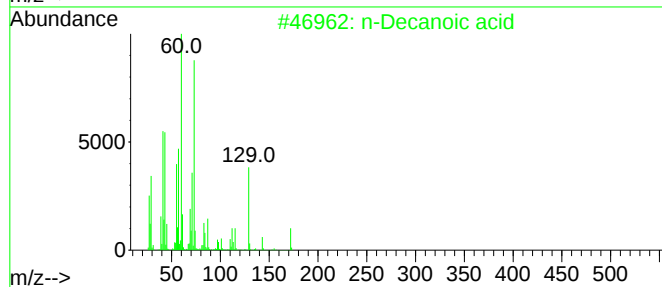
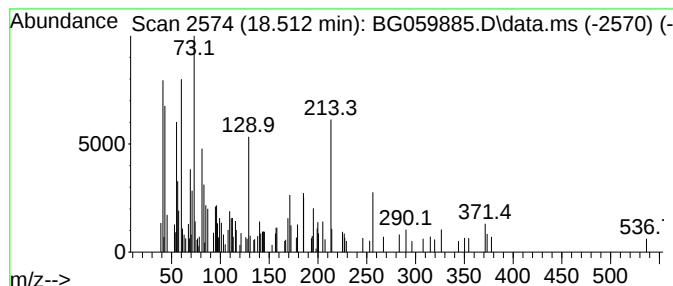
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Decanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.512	2.23 ng	51173	Phenanthrene-d10	17.695

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Decanoic acid	172	C10H20O2	000334-48-5	52
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43
3		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35
4		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	35
5		3,7-Dimethyl-8-oxo-1,5-dioxa-spi...	256	C13H20O5	1000193-79-8	30



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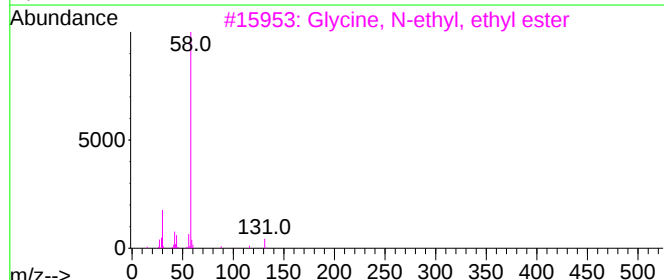
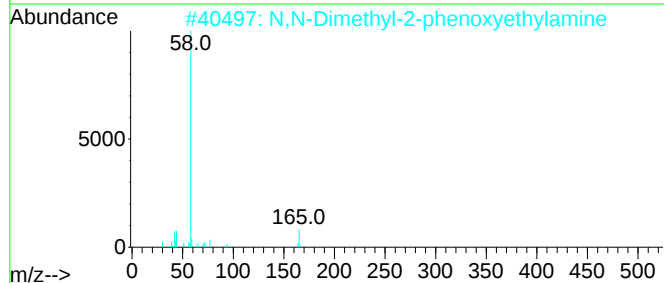
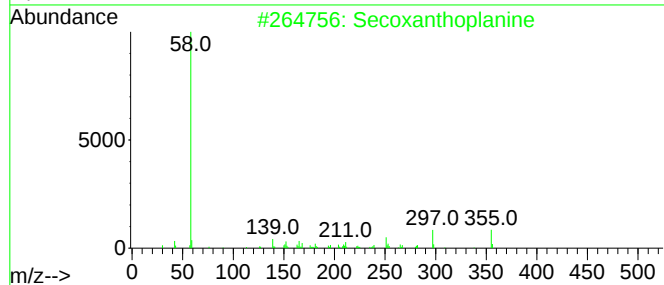
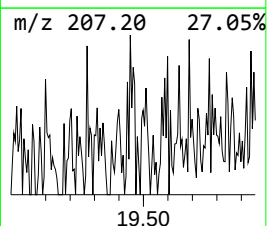
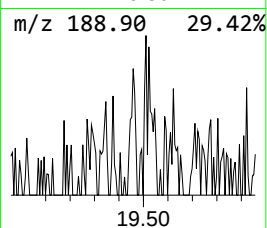
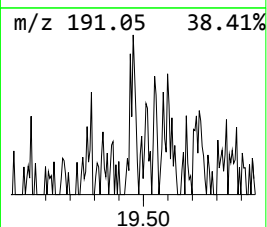
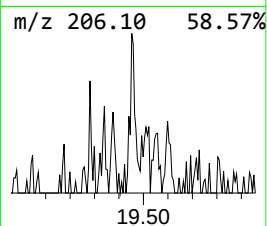
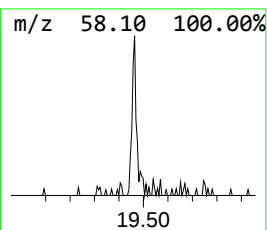
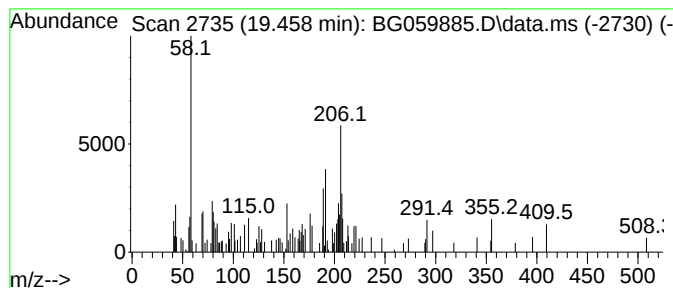
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown19.458 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.458	2.05 ng	47215	Phenanthrene-d10		17.695	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Secoxanthoplanine		355	C21H25NO4	104385-49-1	38
2	N,N-Dimethyl-2-phenoxyethylamine		165	C10H15NO	013468-02-5	25
3	Glycine, N-ethyl, ethyl ester		131	C6H13NO2	1000452-81-1	25
4	1,3-Diphenyl-3-methylcyclopropene		206	C16H14	086544-79-8	25
5	Psilocin		204	C12H16N2O	000520-53-6	25



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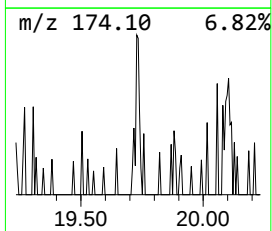
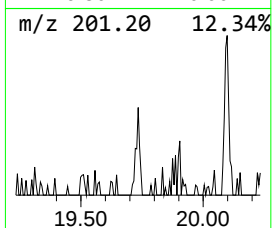
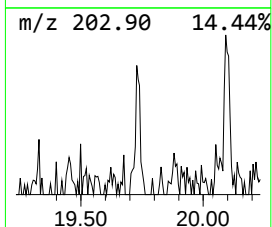
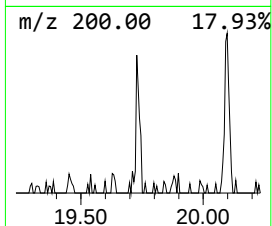
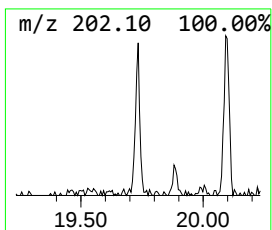
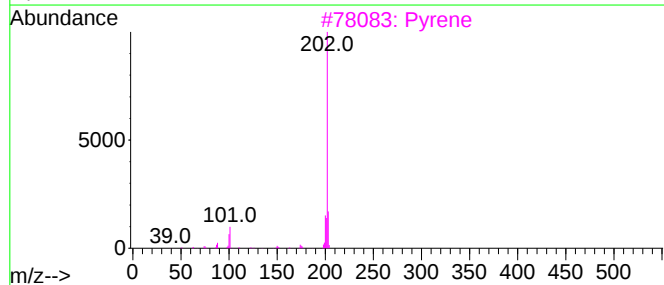
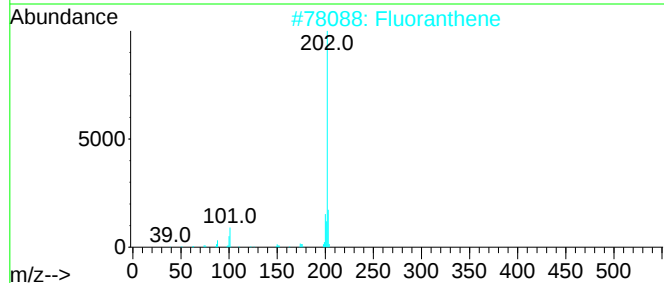
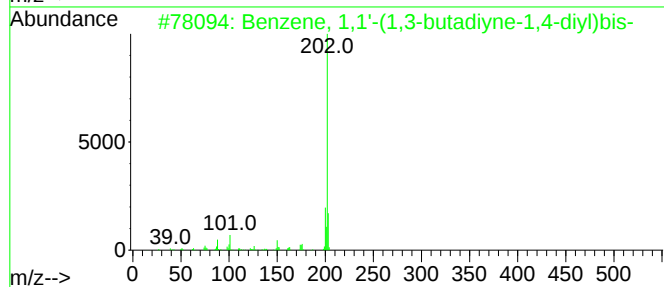
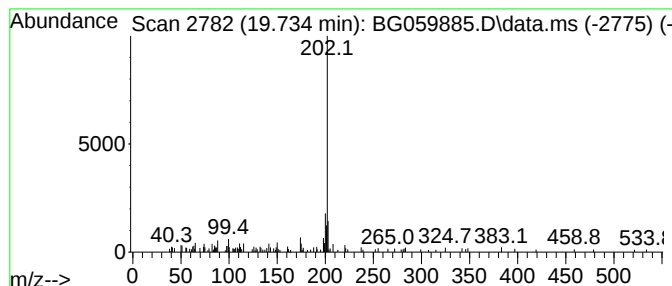
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.734	2.62 ng	60142	Phenanthrene-d10	17.695

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
2			Fluoranthene	202	C16H10	000206-44-0	72
3			Pyrene	202	C16H10	000129-00-0	72
4			L-Tryptophan, 1-(trimethylsilyl)...	348	C17H28N2O2Si2	1033331-59-7	53
5			1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	45



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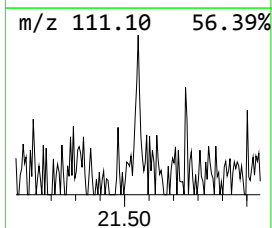
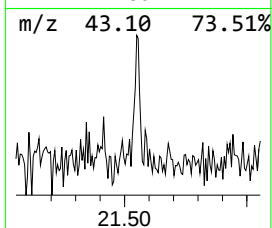
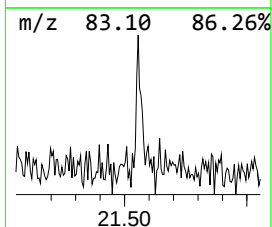
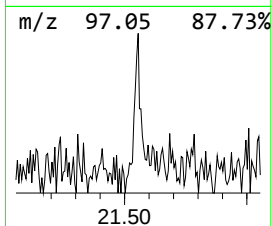
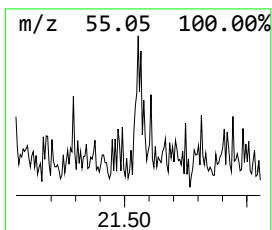
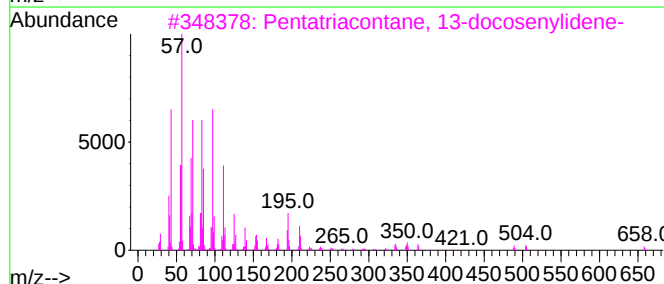
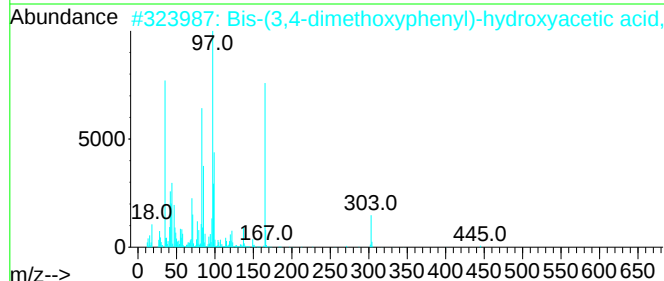
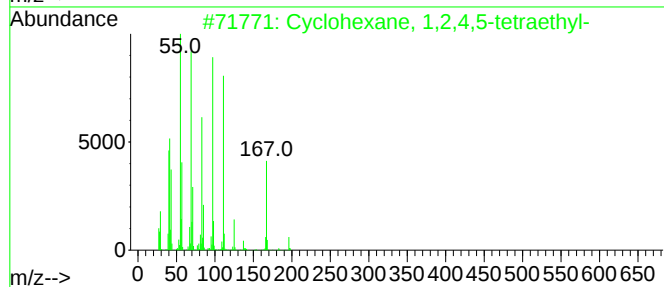
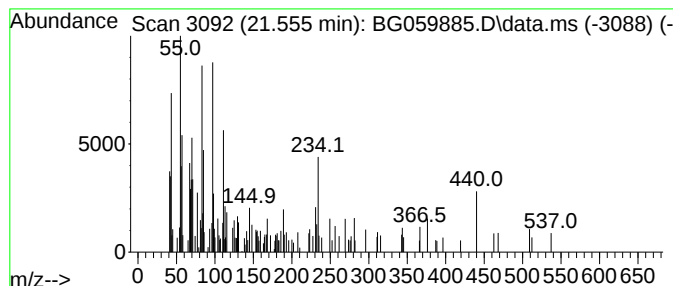
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown21.555 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.555	2.66 ng	61417	Chrysene-d12	22.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2,4,5-tetraethyl-	196	C14H28	061142-00-5	38
2			Bis-(3,4-dimethoxyphenyl)-hydrox...	445	C24H31NO7	095805-62-2	17
3			Pentatriacontane, 13-docosenylid...	659	C47H94	1010156-09-1	10
4			Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	10
5			Tetradecanoic acid, dodecyl ester	396	C26H52O2	002040-64-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059885.D
Acq On : 25 Nov 2023 10:35
Operator : MA/JU
Sample : 05366-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P-13(10-15)

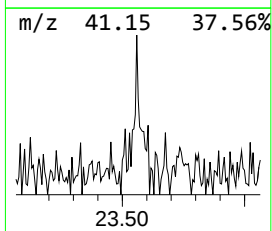
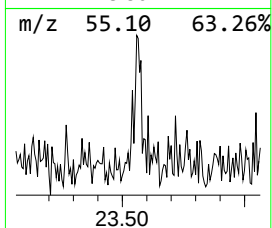
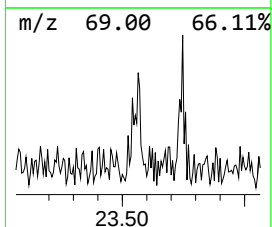
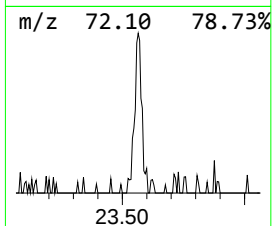
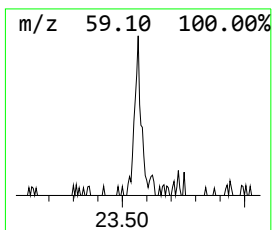
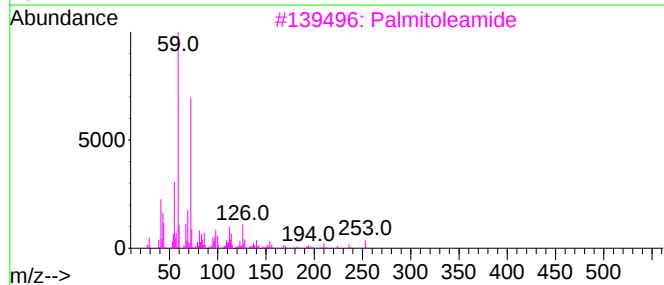
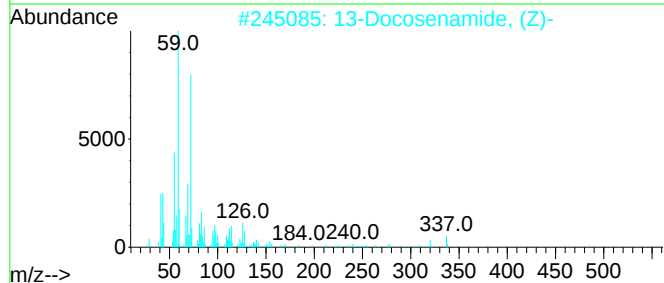
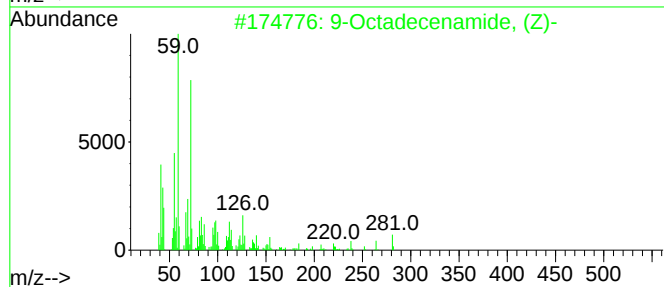
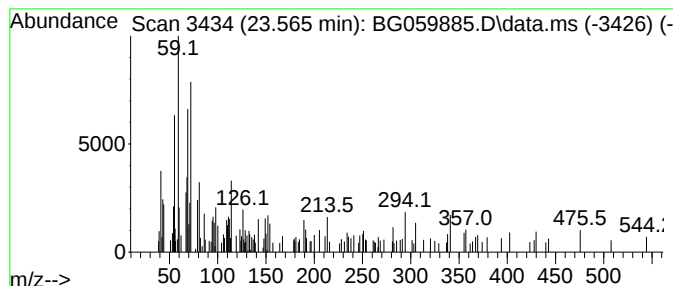
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.565	4.33 ng	99950	Chrysene-d12	22.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-			281	C18H35NO	000301-02-0	86
2	13-Docosenamide, (Z)-			337	C22H43NO	000112-84-5	70
3	Palmitoleamide			253	C16H31NO	106010-22-4	53
4	Isobutyramide, N-(2-pentyl)-N-et...			185	C11H23NO	1000464-57-1	25
5	1-Ethyl-3-piperidinamine, N-trim...			200	C10H24N2Si	1000469-35-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059885.D
Acq On : 25 Nov 2023 10:35
Operator : MA/JU
Sample : 05366-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P-13(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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
2,5-cyclohexadi...	14.622	3.9	ng	83376	3	14.951	425113	20.0
n-Decanoic acid	18.512	2.2	ng	51173	4	17.695	459706	20.0
unknown19.458	19.458	2.0	ng	47215	4	17.695	459706	20.0
Benzene, 1,1'-(...	19.734	2.6	ng	60142	4	17.695	459706	20.0
unknown21.555	21.555	2.7	ng	61417	5	22.019	461894	20.0
9-Octadecenamid...	23.565	4.3	ng	99950	5	22.019	461894	20.0