

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
 Data File : BG059776.D
 Acq On : 20 Nov 2023 19:48
 Operator : MA/JU
 Sample : 05356-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VNJ-205

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: BG059776.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.825	408	415	422	rBV	474369	744787	31.61%	5.231%
2	7.453	684	692	699	rBV	579042	974460	41.35%	6.844%
3	8.334	835	842	848	rBV2	149834	256642	10.89%	1.803%
4	9.527	1037	1045	1052	rBV	371781	656168	27.85%	4.609%
5	11.178	1319	1326	1333	rBV	214481	375139	15.92%	2.635%
6	13.581	1729	1735	1741	rVB	1015026	1493047	63.36%	10.487%
7	13.781	1765	1769	1775	rVB5	17476	31524	1.34%	0.221%
8	14.962	1964	1970	1977	rBV	311204	479006	20.33%	3.364%
9	15.026	1977	1981	1985	rVB3	25242	40793	1.73%	0.287%
10	16.002	2144	2147	2156	rVB3	26008	47259	2.01%	0.332%
11	16.296	2188	2197	2199	rVB8	11666	29782	1.26%	0.209%
12	16.442	2216	2222	2230	rBV	907343	1375982	58.39%	9.665%
13	17.147	2338	2342	2346	rBV7	13975	23813	1.01%	0.167%
14	17.330	2369	2373	2376	rBV5	22761	38145	1.62%	0.268%
15	17.712	2432	2438	2442	rBV2	390582	600711	25.49%	4.219%
16	17.753	2442	2445	2451	rVB	186302	263455	11.18%	1.850%
17	17.841	2457	2460	2467	rVB3	30452	49710	2.11%	0.349%
18	18.017	2486	2490	2493	rBV4	37547	47392	2.01%	0.333%
19	18.111	2503	2506	2512	rVB7	28132	35503	1.51%	0.249%
20	18.405	2552	2556	2563	rVB9	25596	56952	2.42%	0.400%
21	18.528	2572	2577	2582	rBV2	168154	233517	9.91%	1.640%
22	18.628	2590	2594	2597	rVB4	32205	46902	1.99%	0.329%
23	18.775	2612	2619	2622	rBV7	34694	73463	3.12%	0.516%
24	18.939	2644	2647	2650	rVB3	37669	43866	1.86%	0.308%
25	19.116	2674	2677	2683	rBV8	25225	39704	1.68%	0.279%
26	19.421	2726	2729	2730	rBV3	23586	23840	1.01%	0.167%
27	19.462	2733	2736	2739	rBV4	32075	44416	1.88%	0.312%
28	19.633	2758	2765	2768	rBV9	37074	79072	3.36%	0.555%
29	19.744	2778	2784	2788	rBV	283408	392199	16.64%	2.755%
30	19.786	2788	2791	2798	rVB7	57717	88355	3.75%	0.621%
31	19.962	2818	2821	2824	rVB5	52923	54181	2.30%	0.381%
32	20.068	2835	2839	2842	rBV5	55269	80203	3.40%	0.563%
33	20.109	2842	2846	2850	rVV	208150	290496	12.33%	2.040%
34	20.162	2853	2855	2860	rVB6	29228	32507	1.38%	0.228%
35	20.285	2870	2876	2885	rBV	1884992	2356419	100.00%	16.551%
36	20.949	2984	2989	2990	rBV3	269143	387804	16.46%	2.724%

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37	21.049	3003	3006	3013	rVB9	35763	54571	2.32%	0.383%
38	21.378	3060	3062	3066	rVB5	35816	44788	1.90%	0.315%
39	21.578	3093	3096	3102	rVB8	64753	89949	3.82%	0.632%
40	21.748	3121	3125	3127	rBV5	27261	40493	1.72%	0.284%
41	22.036	3167	3174	3179	rVV3	289332	583015	24.74%	4.095%
42	22.089	3179	3183	3188	rVB2	75752	126930	5.39%	0.892%
43	22.559	3258	3263	3270	rBV2	66526	116137	4.93%	0.816%
44	23.452	3412	3415	3425	rVB10	59436	145092	6.16%	1.019%
45	23.599	3436	3440	3442	rBV5	89734	127209	5.40%	0.893%
46	24.457	3581	3586	3592	rBV7	67681	181045	7.68%	1.272%
47	25.620	3776	3784	3793	rVB2	159225	466884	19.81%	3.279%
48	25.861	3817	3825	3829	rBV10	63615	160379	6.81%	1.126%
49	27.177	4047	4049	4054	rVB6	34545	41985	1.78%	0.295%
50	27.330	4072	4075	4077	rBV4	27966	36543	1.55%	0.257%
51	27.482	4097	4101	4102	rBV4	43068	54897	2.33%	0.386%
52	27.905	4170	4173	4174	rBV3	23999	28144	1.19%	0.198%
53	29.415	4428	4430	4432	rBV3	24143	24172	1.03%	0.170%
54	32.494	4952	4954	4957	rBV4	20391	28016	1.19%	0.197%

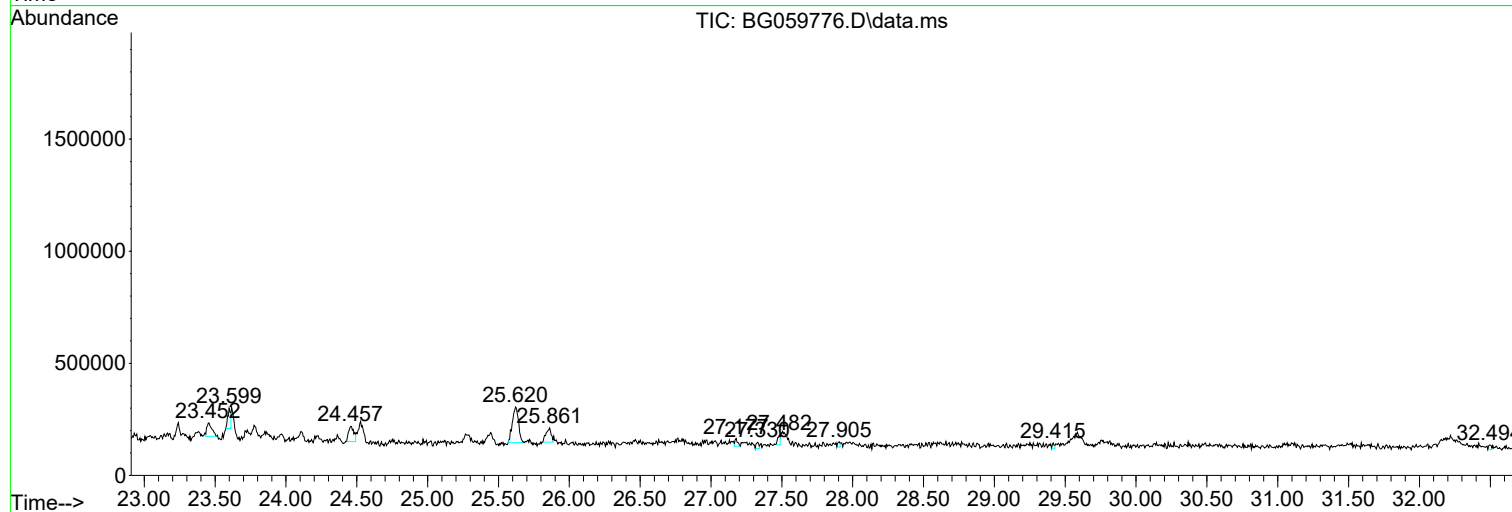
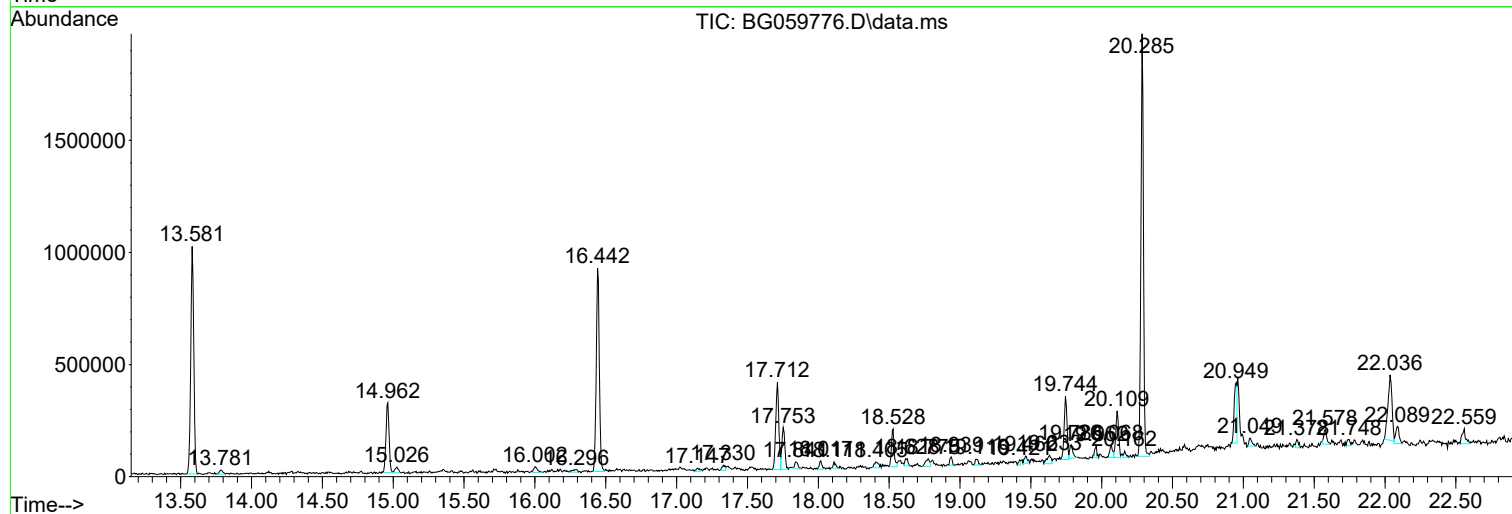
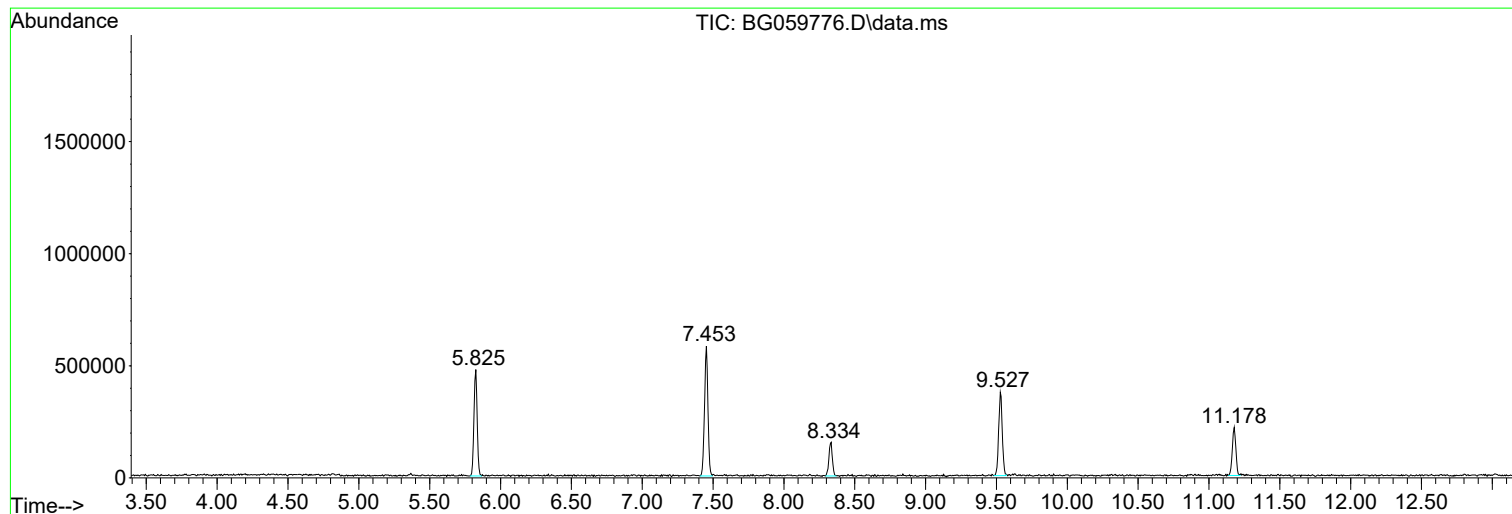
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Acq On : 20 Nov 2023 19:48
Operator : MA/JU
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VNJ-205

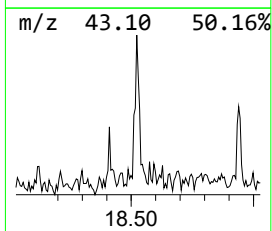
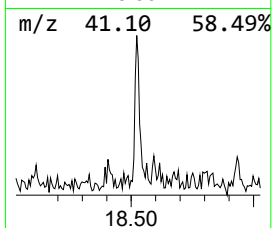
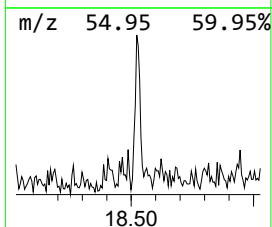
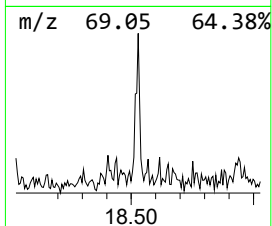
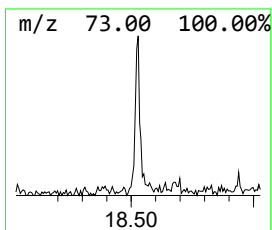
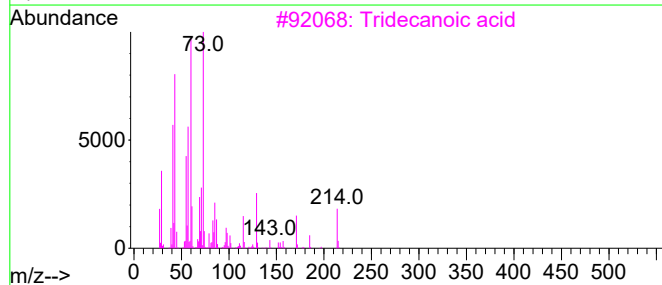
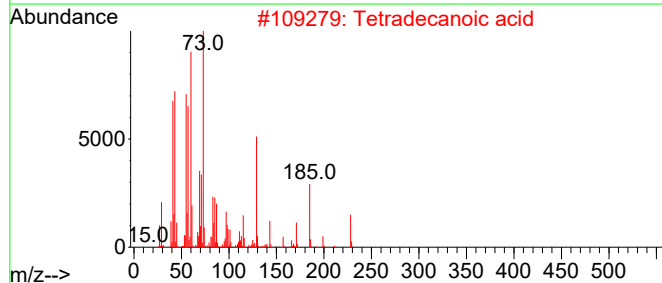
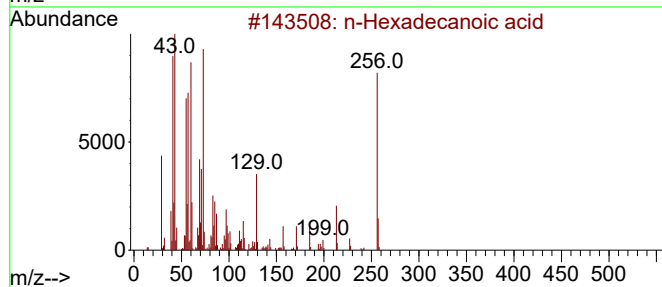
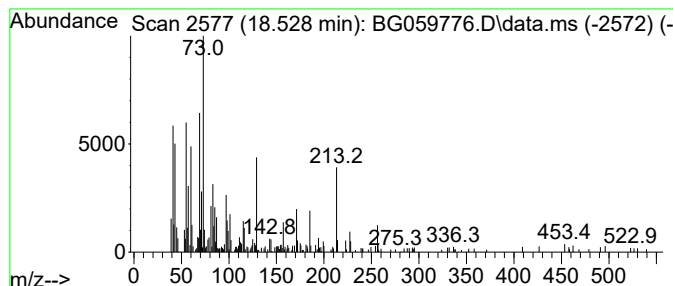
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.528	7.77 ng	233517	Phenanthrene-d10	17.712

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	47
3			Tridecanoic acid	214	C13H26O2	000638-53-9	45
4			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	38
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	38



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Misc :
ALS Vial : 10 Sample Multiplier: 1

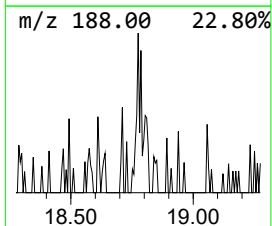
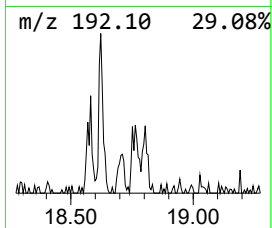
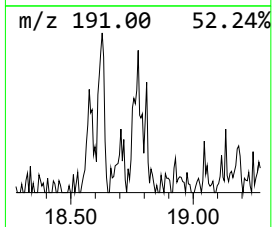
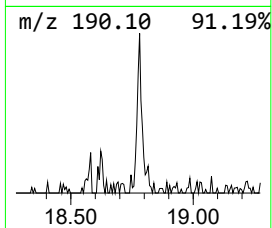
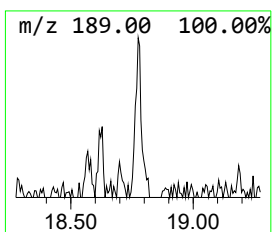
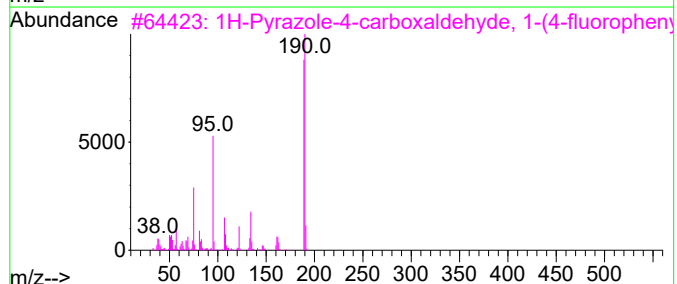
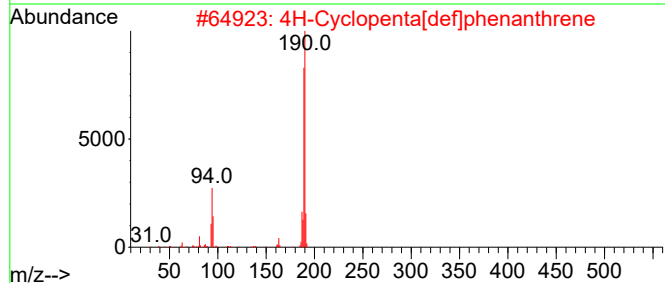
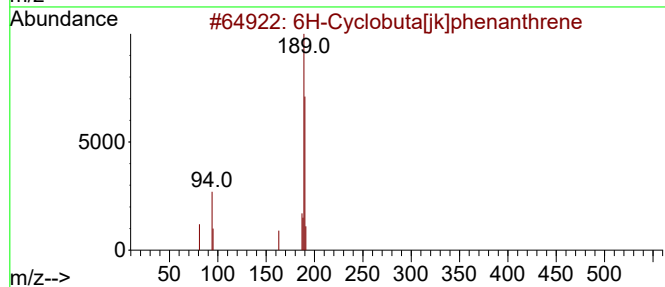
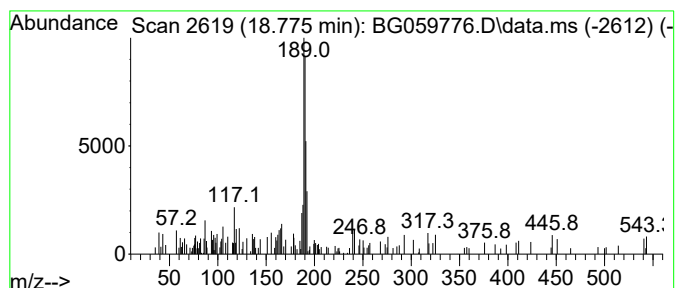
Instrument :
BNA_G
ClientSampleId :
VNJ-205

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 2 6H-Cyclobuta[jk]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.775	2.45 ng	73463	Phenanthrene-d10	17.712	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	52
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	50
3	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	49
4	3-(Trifluoromethoxy)benzaldehyde	190	C8H5F3O2	052771-21-8	47
5	2-Chloro-4,6-difluoroaniline, N,...	191	C8H8ClF2N	943830-85-1	43



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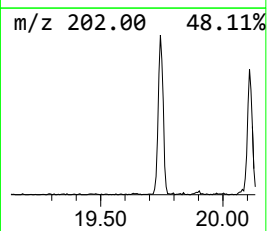
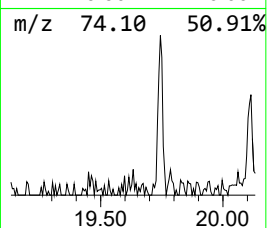
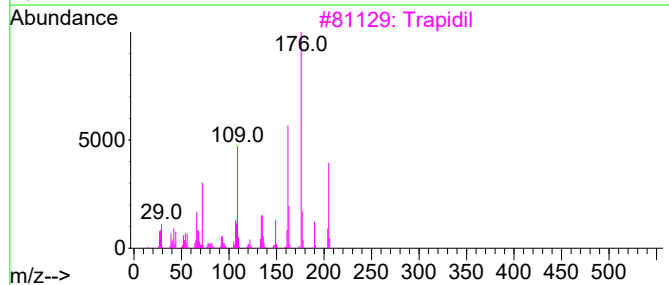
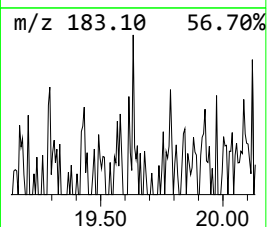
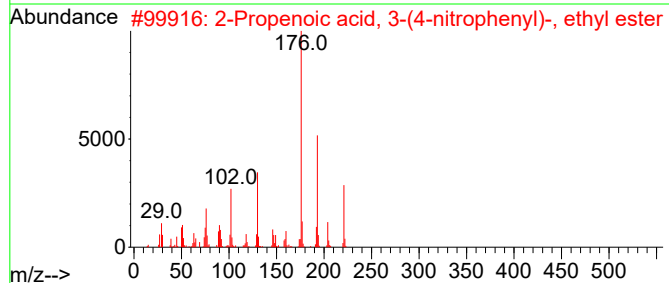
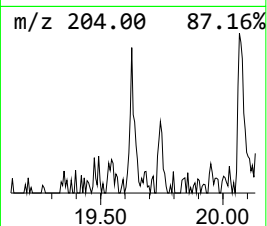
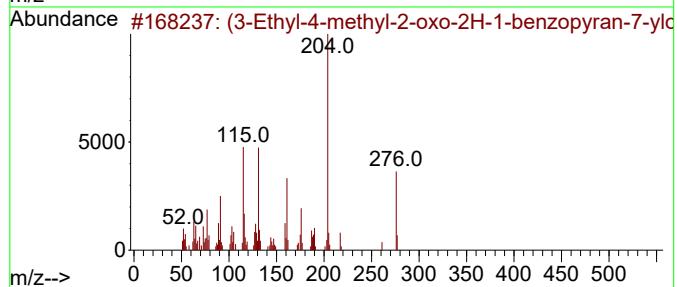
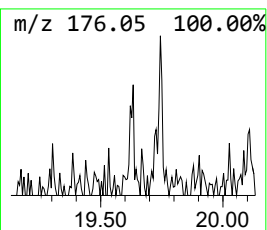
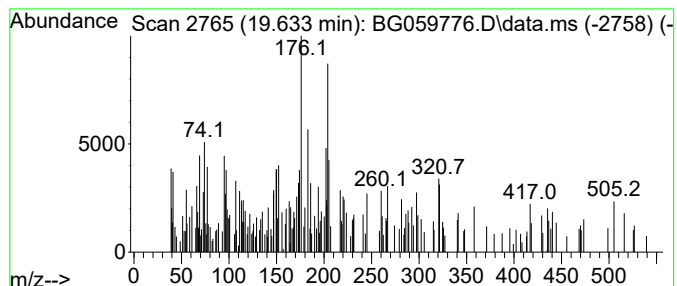
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown19.633 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.633	2.63 ng	79072	Phenanthrene-d10	17.712

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(3-Ethyl-4-methyl-2-oxo-2H-1-ben...	276	C14H16N2O4	1000442-14-1	14
2			2-Propenoic acid, 3-(4-nitrophen...	221	C11H11NO4	000953-26-4	14
3			Trapidil	205	C10H15N5	015421-84-8	11
4			Pyrido[2,3-d]pyrimidine-4(3H)-on...	176	C8H8N4O	049739-04-0	11
5			Benzofurane-2-carboxamide, 3-amino-	176	C9H8N2O2	054802-10-7	11



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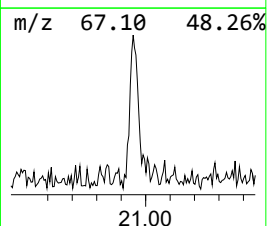
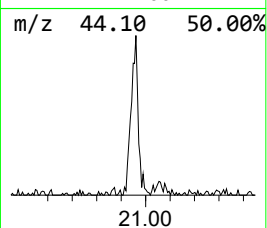
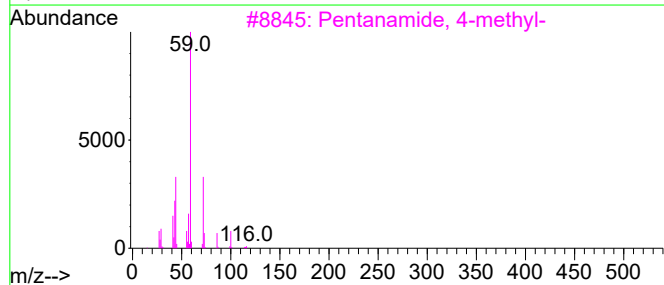
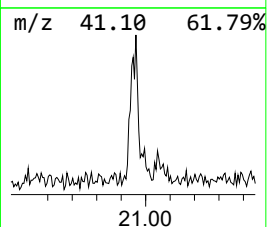
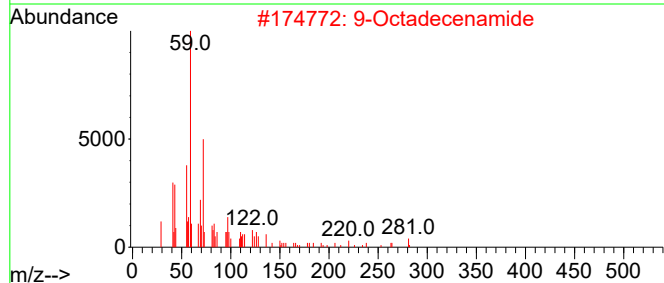
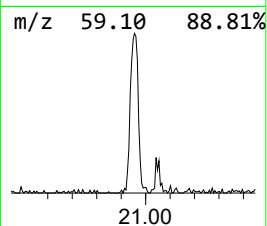
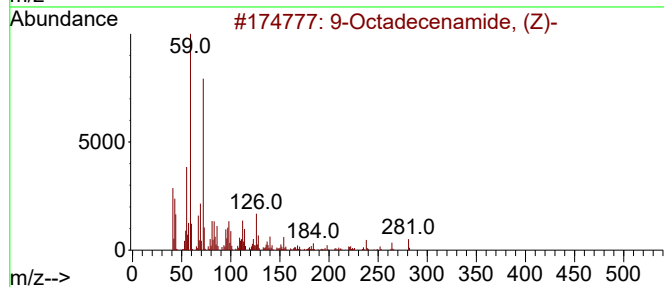
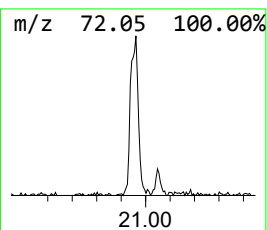
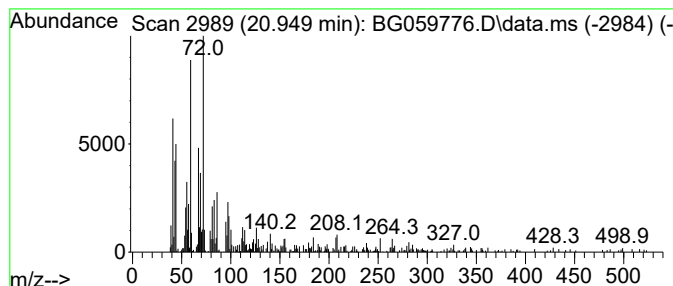
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.949	13.30 ng	387804	Chrysene-d12	22.036

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	66
2			9-Octadecenamide	281	C18H35NO	003322-62-1	41
3			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	38
4			N-Formyl-.alpha.-alanine	159	C7H13NO3	1000222-03-5	27
5			1-(4-ethoxyphenyl)-N-ethylpropan...	207	C13H21NO	1000455-82-7	27



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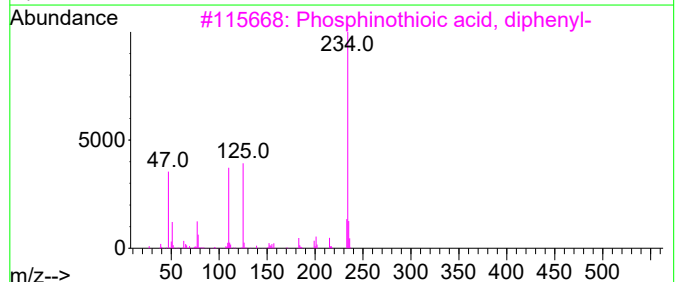
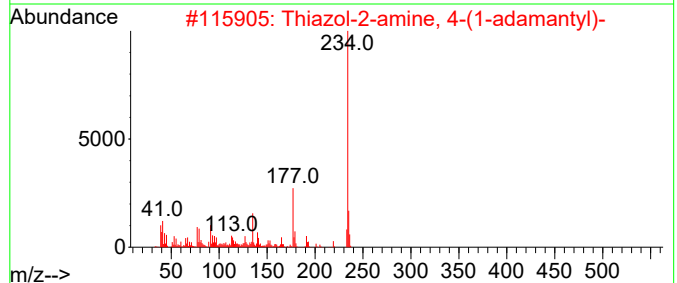
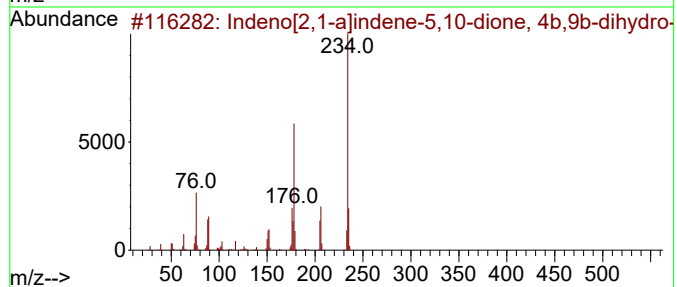
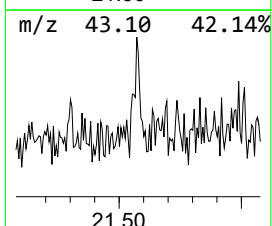
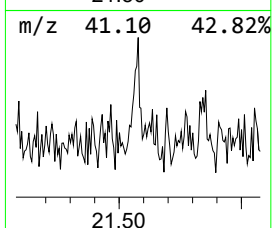
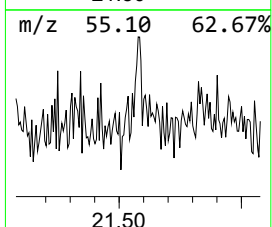
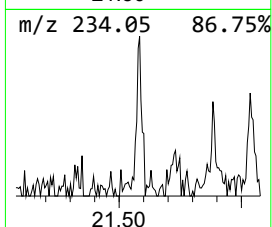
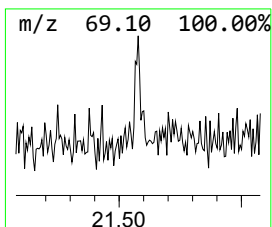
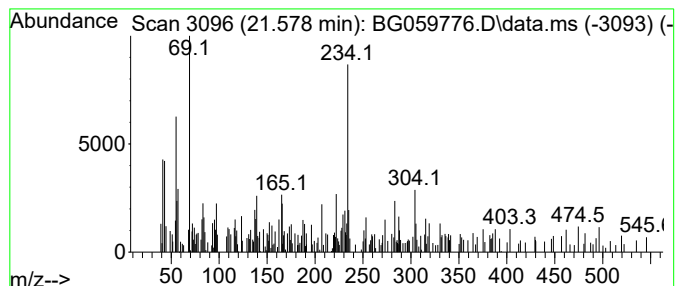
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown21.578 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.578	3.09 ng	89949	Chrysene-d12	22.036

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indeno[2,1-a]indene-5,10-dione, ...	234	C16H10O2	050703-54-3	46
2			Thiazol-2-amine, 4-(1-adamantyl)-	234	C13H18N2S	019735-74-1	46
3			Phosphinothioic acid, diphenyl-	234	C12H11OPS	014278-72-9	46
4			2-Phenyl-6,7-dimethylquinoxaline	234	C16H14N2	071897-07-9	46
5			3-Nitroaniline, N-trifluoroacetyl-	234	C8H5F3N2O3	025080-83-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059776.D
Acq On : 20 Nov 2023 19:48
Operator : MA/JU
Sample : 05356-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

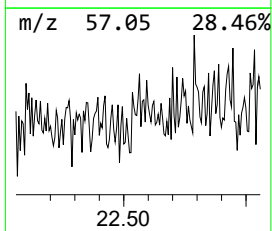
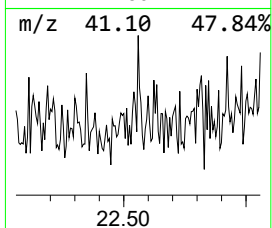
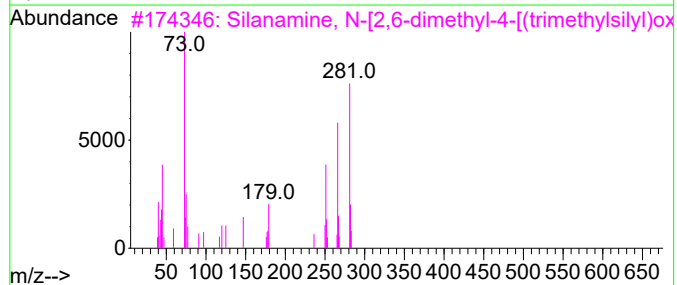
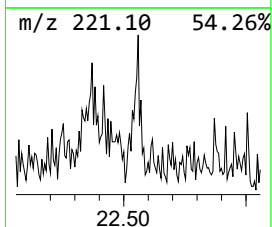
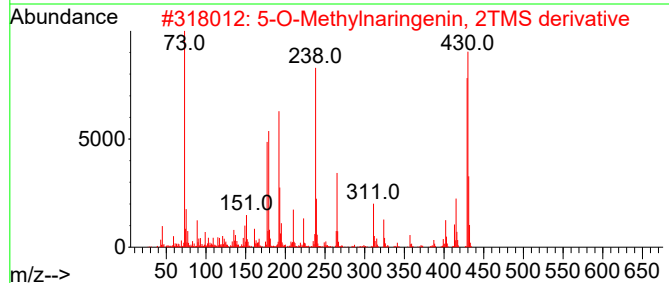
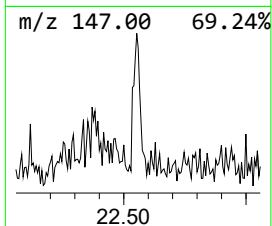
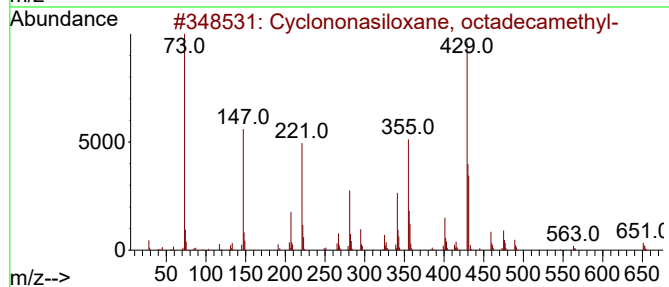
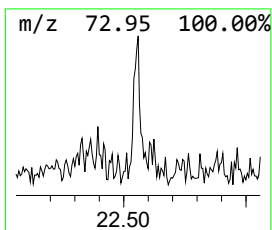
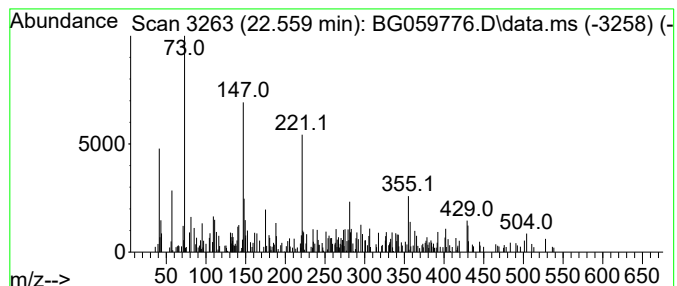
Instrument :
BNA_G
ClientSampleId :
VNJ-205

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 6 unknown22.559 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.559	3.98 ng	116137	Chrysene-d12		22.036	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-		666	C18H54O9Si9	000556-71-8	47
2	5-O-Methylnaringenin, 2TMS deriv...		430	C22H30O5Si2	1000488-69-0	11
3	Silanamine, N-[2,6-dimethyl-4-[(...		281	C14H27NOSi2	072088-09-6	11
4	N-Benzyl-N-ethyl-p-isopropylbenz...		281	C19H23NO	015089-22-2	11
5	Hexasiloxane, tetradecamethyl-		458	C14H42O5Si6	000107-52-8	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059776.D
Acq On : 20 Nov 2023 19:48
Operator : MA/JU
Sample : 05356-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-205

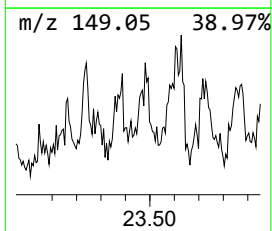
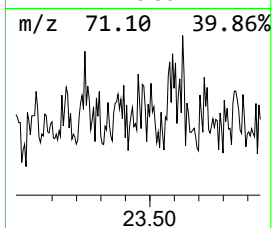
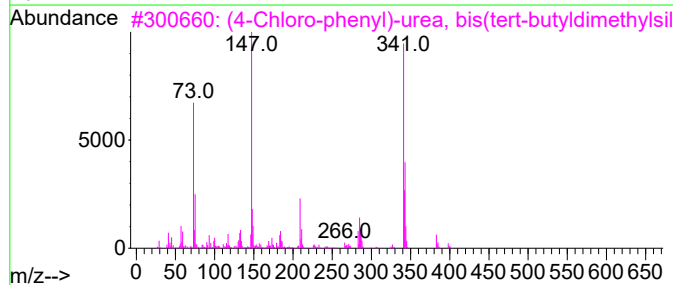
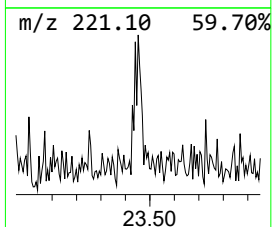
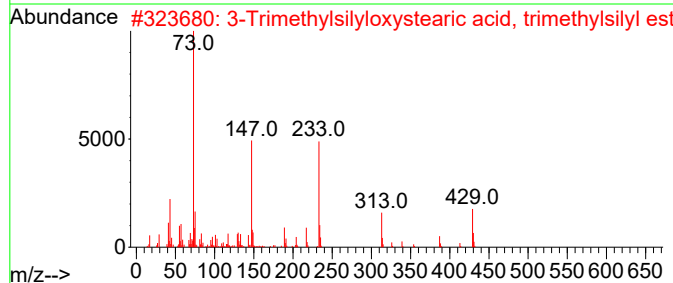
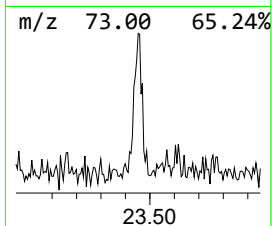
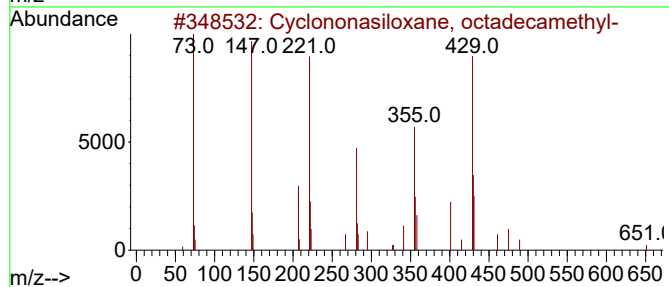
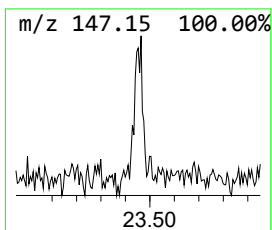
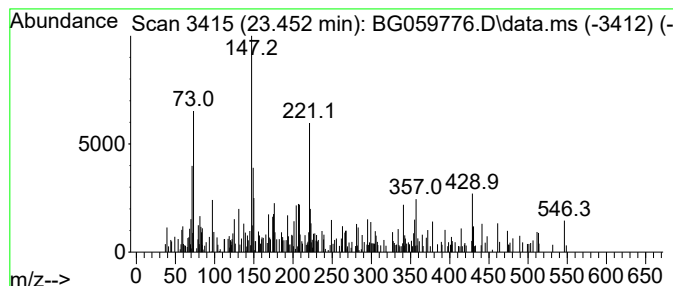
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown23.452 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.452	4.98 ng	145092	Chrysene-d12	22.036

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	36
2			3-Trimethylsilyloxystearic acid,...	444	C24H52O3Si2	1000079-42-6	28
3			(4-Chloro-phenyl)-urea, bis(tert...	398	C19H35ClN2O5Si2	1000385-82-2	27
4			2,2,2-Trifluoro-N-{2-hydroxy-3-[...	498	C16H32F6N2O3Si3	1000475-04-0	25
5			D-Xylulose, tetrakis(trimethylsi...	633	C24H44F5N5O5Si4	1000394-61-3	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059776.D
Acq On : 20 Nov 2023 19:48
Operator : MA/JU
Sample : 05356-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

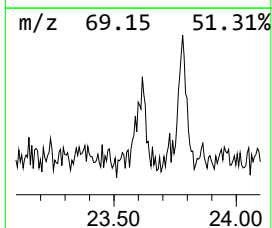
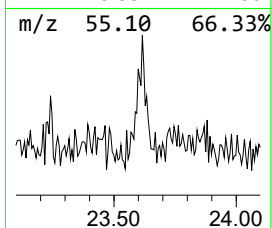
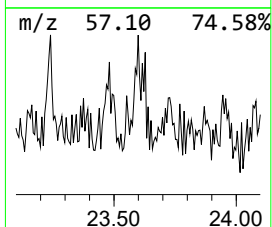
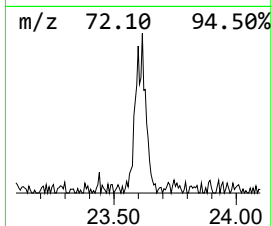
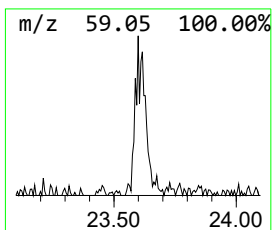
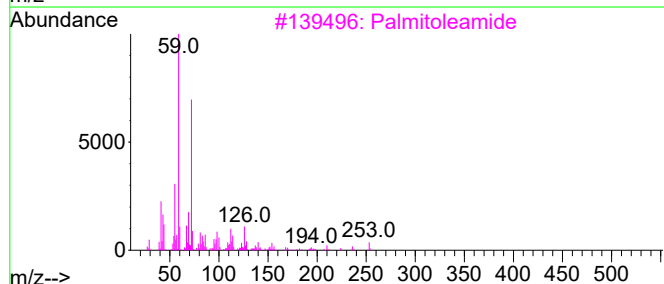
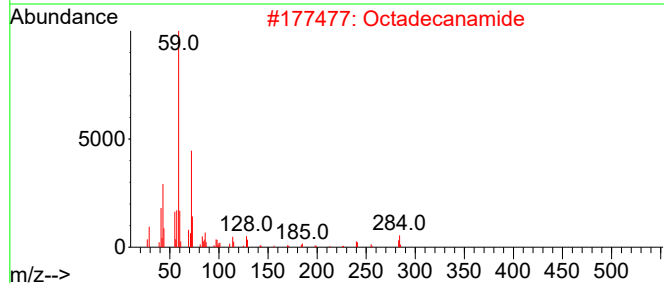
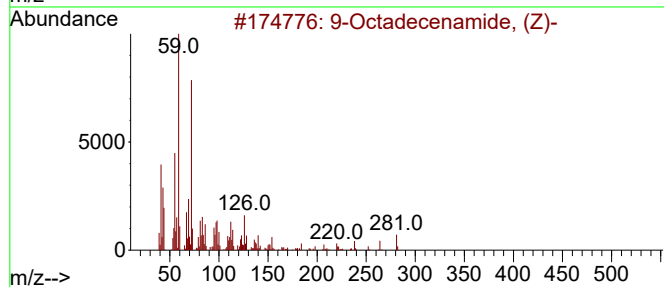
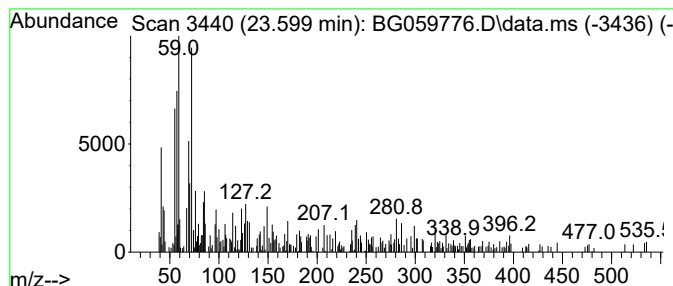
Instrument :
BNA_G
ClientSampleId :
VNJ-205

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

Peak Number 8 Octadecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.599	4.36 ng	127209	Chrysene-d12	22.036	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	81
2	Octadecanamide	283	C18H37NO	000124-26-5	74
3	Palmitoleamide	253	C16H31NO	106010-22-4	74
4	Nonadecanamide	297	C19H39NO	058185-32-3	50
5	Behenic amide	339	C22H45NO	003061-75-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059776.D
Acq On : 20 Nov 2023 19:48
Operator : MA/JU
Sample : 05356-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

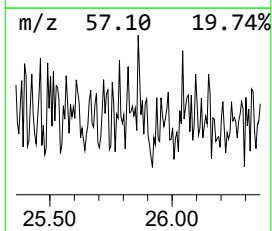
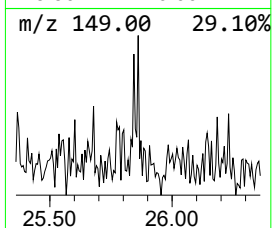
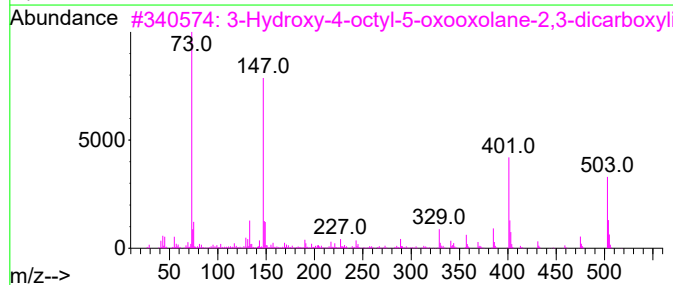
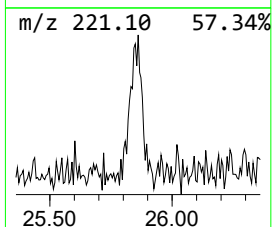
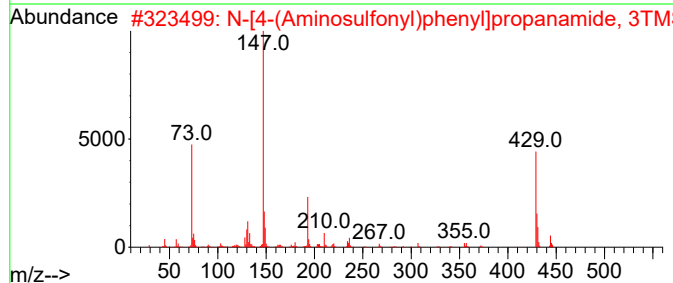
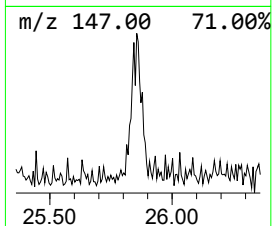
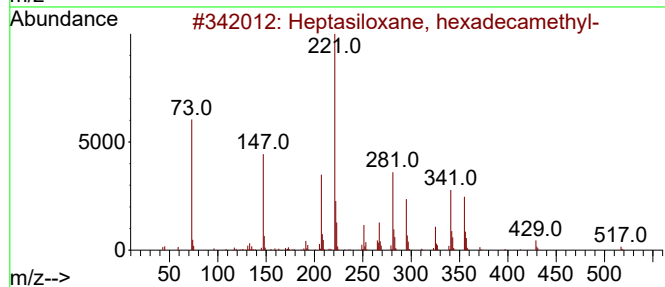
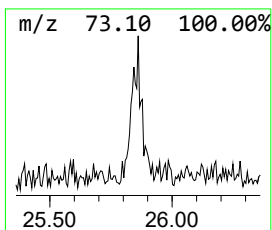
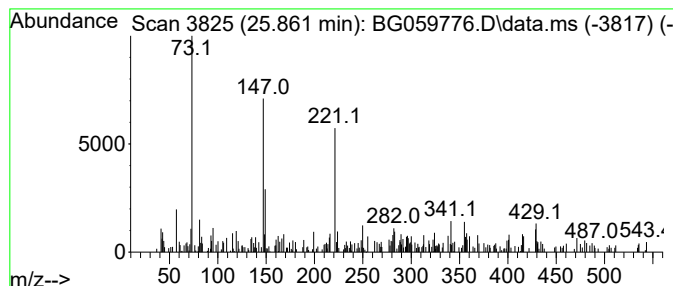
Instrument :
BNA_G
ClientSampleId :
VNJ-205

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

Peak Number 9 unknown25.861 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.861	6.87 ng	160379	Perylene-d12	25.626	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
2	N-[4-(Aminosulfonyl)phenyl]propa...	444	C18H36N2O3SSi3	1000500-82-8	32
3	3-Hydroxy-4-octyl-5-oxoxolane-2...	518	C23H46O7Si3	1000503-31-2	22
4	Trimethylsilyl [2-(4-chloropheny...	401	C20H20ClNO2SSi	1000408-26-6	22
5	[(5-Fluoro-1H-indol-2-yl)methyl]...	322	C16H27FN2Si2	1000504-51-1	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059776.D
Acq On : 20 Nov 2023 19:48
Operator : MA/JU
Sample : 05356-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

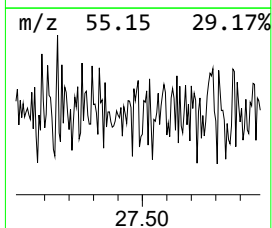
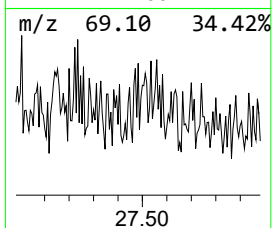
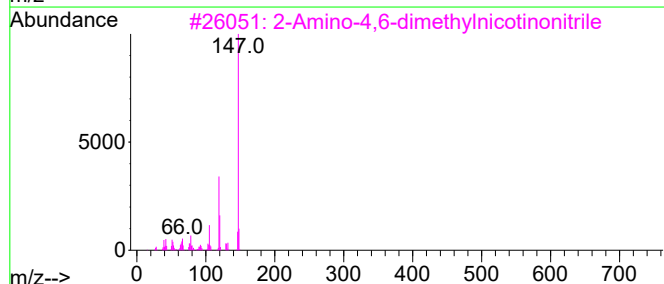
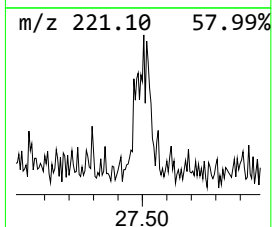
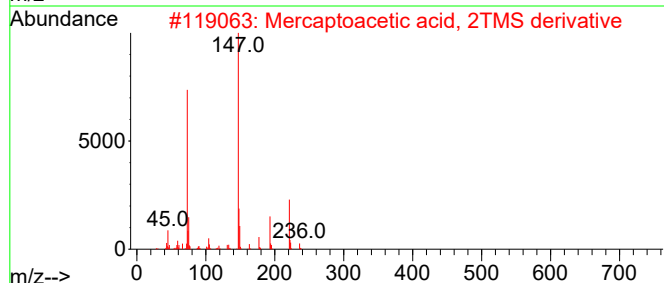
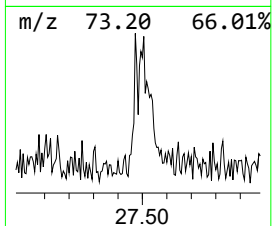
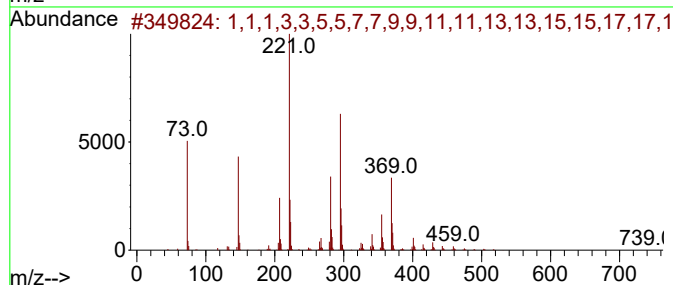
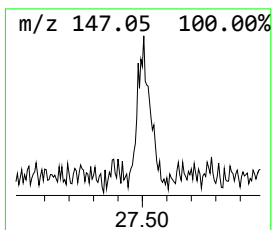
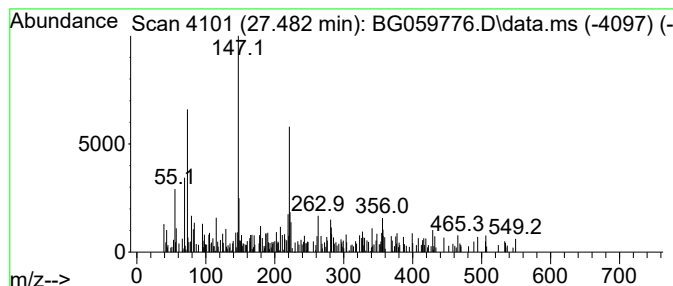
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,1,1,3,3,5,5,7,7,9,9,11,11... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
27.482	2.35 ng	54897	Perylene-d12	25.626	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	53
2	Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	50
3	2-Amino-4,6-dimethylnicotinonitrile	147	C8H9N3	005468-34-8	27
4	But-2-enoic acid, 2-hydroxy-4-ox...	359	C17H14BrNO3	1000310-69-6	27
5	N-(Hydroxymethyl)-2-methylprop-2...	259	C11H25NO2Si2	1000511-32-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059776.D
Acq On : 20 Nov 2023 19:48
Operator : MA/JU
Sample : 05356-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-205

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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
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6H-Cyclobuta[jk...	18.775	2.5	ng	73463	4	17.712	600711	20.0
unknown19.633	19.633	2.6	ng	79072	4	17.712	600711	20.0
9-Octadecenamid...	20.949	13.3	ng	387804	5	22.036	583015	20.0
unknown21.578	21.578	3.1	ng	89949	5	22.036	583015	20.0
unknown22.559	22.559	4.0	ng	116137	5	22.036	583015	20.0
unknown23.452	23.452	5.0	ng	145092	5	22.036	583015	20.0
Octadecanamide	23.599	4.4	ng	127209	5	22.036	583015	20.0
unknown25.861	25.861	6.9	ng	160379	6	25.626	466884	20.0
1,1,1,3,3,5,5,7...	27.482	2.4	ng	54897	6	25.626	466884	20.0