

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
 Data File : BG059780.D
 Acq On : 20 Nov 2023 22:30
 Operator : MA/JU
 Sample : 05376-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 210

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: BG059780.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.367	334	337	342	rVB4	12828	17976	1.11%	0.155%
2	5.825	408	415	422	rVB	335147	558728	34.55%	4.827%
3	7.453	681	692	702	rBV2	434365	750496	46.41%	6.483%
4	8.334	833	842	849	rBV2	176126	303524	18.77%	2.622%
5	9.527	1040	1045	1052	rVB2	290298	530787	32.83%	4.585%
6	11.184	1319	1327	1332	rBV2	224536	411011	25.42%	3.551%
7	12.811	1598	1604	1608	rBV3	19668	34889	2.16%	0.301%
8	13.029	1638	1641	1645	rVB4	17491	17983	1.11%	0.155%
9	13.581	1729	1735	1742	rBV	809458	1266069	78.30%	10.937%
10	13.704	1750	1756	1758	rBV5	10487	16634	1.03%	0.144%
11	13.792	1765	1771	1777	rVB	369471	566750	35.05%	4.896%
12	14.133	1826	1829	1832	rVB5	16095	21338	1.32%	0.184%
13	14.333	1859	1863	1869	rVB7	13933	27015	1.67%	0.233%
14	14.509	1887	1893	1896	rBV6	8872	16995	1.05%	0.147%
15	14.691	1922	1924	1930	rVB3	14417	17168	1.06%	0.148%
16	14.962	1964	1970	1976	rVB2	366276	577837	35.73%	4.992%
17	15.032	1976	1982	1985	rVB8	11217	18979	1.17%	0.164%
18	15.408	2044	2046	2050	rVB4	20084	23363	1.44%	0.202%
19	15.555	2065	2071	2072	rBV4	13989	20224	1.25%	0.175%
20	15.714	2095	2098	2105	rVB9	14804	25854	1.60%	0.223%
21	16.002	2145	2147	2151	rVB5	13155	16323	1.01%	0.141%
22	16.448	2215	2223	2232	rBV2	717304	1124829	69.56%	9.717%
23	16.924	2302	2304	2310	rVB5	21662	29464	1.82%	0.255%
24	17.230	2354	2356	2358	rVB3	20124	16298	1.01%	0.141%
25	17.259	2358	2361	2364	rBV5	15453	21072	1.30%	0.182%
26	17.377	2375	2381	2384	rBV7	16004	33509	2.07%	0.289%
27	17.418	2384	2388	2391	rVB6	14505	22863	1.41%	0.198%
28	17.711	2433	2438	2443	rBV	433891	685513	42.39%	5.922%
29	17.758	2443	2446	2451	rVB2	106490	157424	9.74%	1.360%
30	17.852	2457	2462	2467	rBV2	35608	61101	3.78%	0.528%
31	17.911	2470	2472	2476	rBV5	13485	17939	1.11%	0.155%
32	18.105	2503	2505	2507	rBV3	13898	17132	1.06%	0.148%
33	18.217	2523	2524	2529	rVB5	19757	20190	1.25%	0.174%
34	18.522	2573	2576	2580	rVB6	45019	54285	3.36%	0.469%
35	18.581	2582	2586	2589	rVV3	31976	45850	2.84%	0.396%
36	18.628	2590	2594	2597	rVB2	48507	58948	3.65%	0.509%

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37	18.698	2603	2606	2607	rBV3	29493	30728	1.90%	0.265%
38	18.763	2614	2617	2620	rBV4	54943	62603	3.87%	0.541%
39	18.939	2645	2647	2649	rBV2	14950	16722	1.03%	0.144%
40	19.069	2665	2669	2671	rBV5	25889	26502	1.64%	0.229%
41	19.127	2675	2679	2681	rBV5	35134	43491	2.69%	0.376%
42	19.180	2686	2688	2690	rBV3	28482	27336	1.69%	0.236%
43	19.468	2734	2737	2742	rBV6	55316	78895	4.88%	0.682%
44	19.750	2780	2785	2791	rBV2	251673	373279	23.08%	3.225%
45	20.109	2842	2846	2852	rBV	252719	342733	21.20%	2.961%
46	20.291	2872	2877	2882	rVB	1223076	1617006	100.00%	13.969%
47	22.042	3168	3175	3180	rBV2	316216	632751	39.13%	5.466%
48	22.559	3258	3263	3267	rVB4	74156	129192	7.99%	1.116%
49	23.452	3411	3415	3423	rVB7	100999	188168	11.64%	1.626%
50	25.855	3818	3824	3836	rVB7	107745	356439	22.04%	3.079%
51	32.441	4943	4945	4948	rBV4	36061	43657	2.70%	0.377%

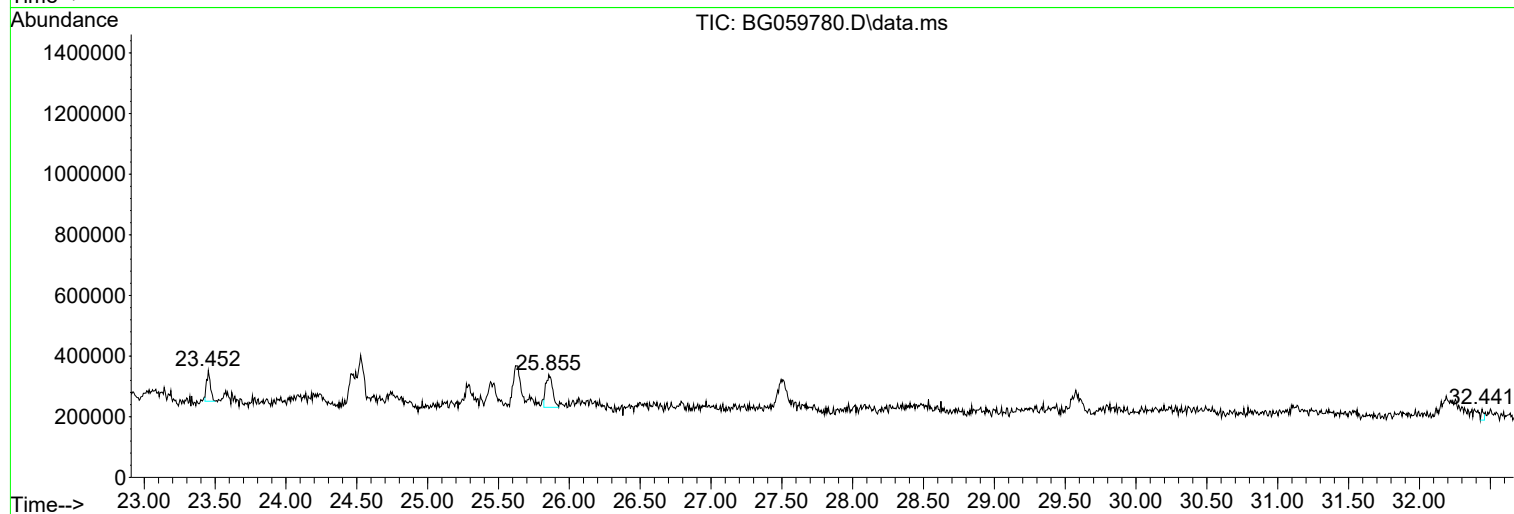
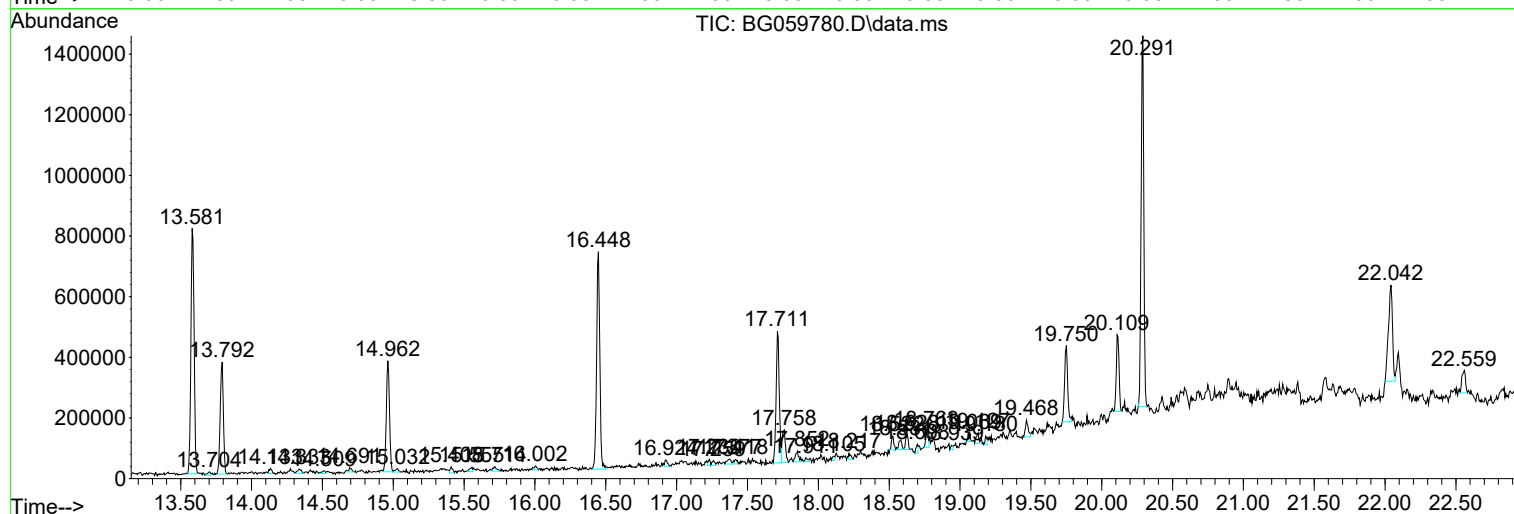
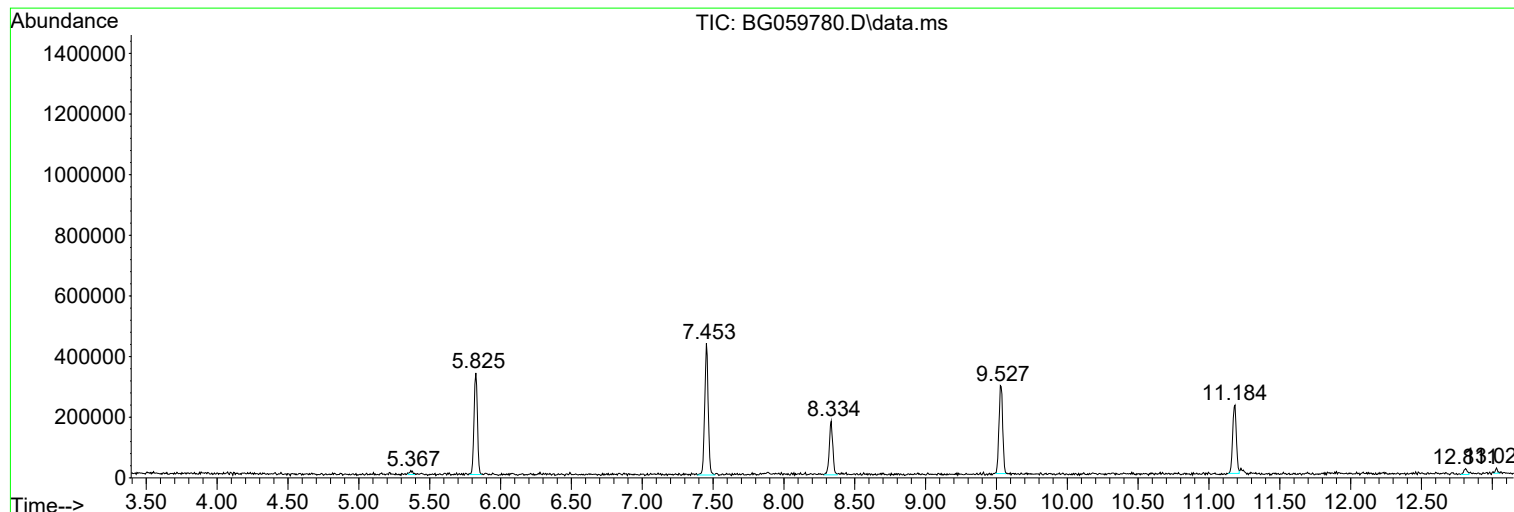
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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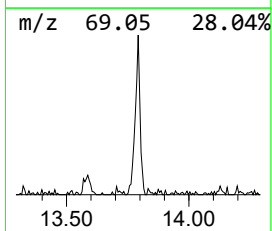
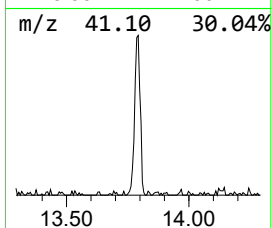
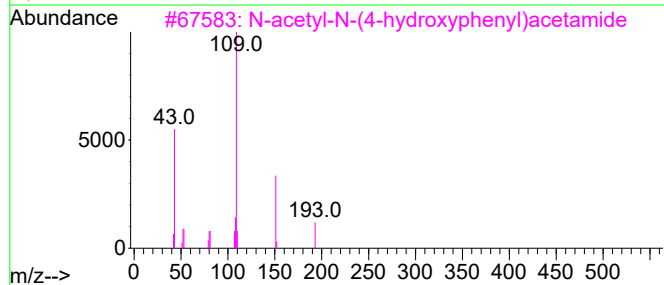
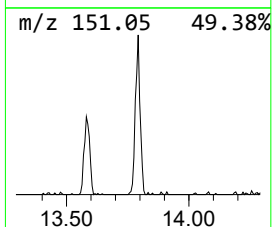
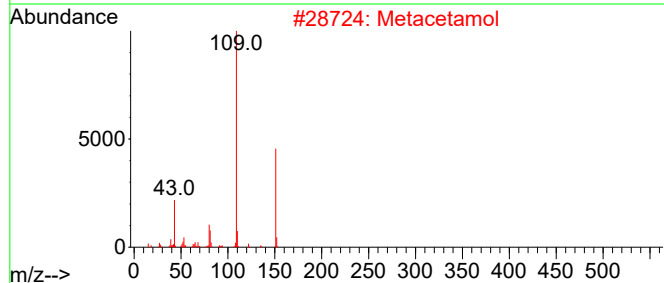
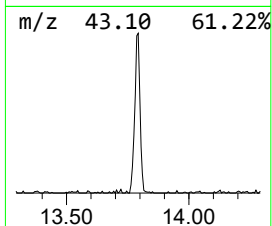
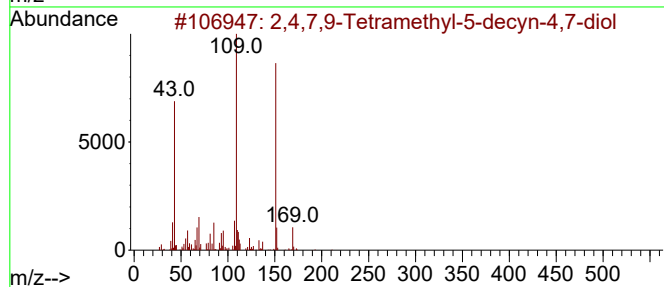
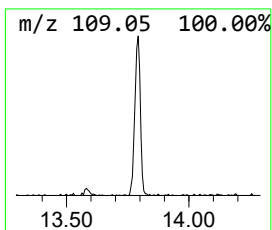
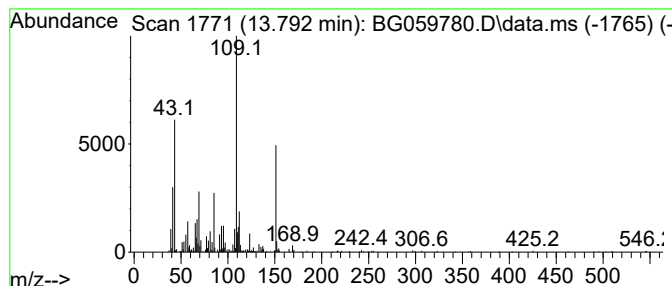
Instrument :
BNA_G
ClientSampleId :
210

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 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.793	19.62 ng	566750	Acenaphthene-d10	14.962	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	64
2	Metacetamol	151	C8H9NO2	000621-42-1	58
3	N-acetyl-N-(4-hydroxyphenyl)acet...	193	C10H11NO3	1000389-51-9	53
4	Diacetamate	193	C10H11NO3	002623-33-8	53
5	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	53



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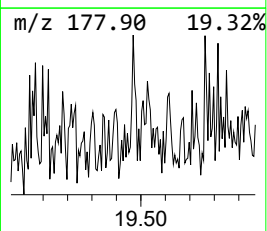
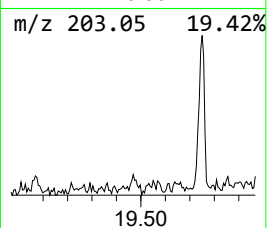
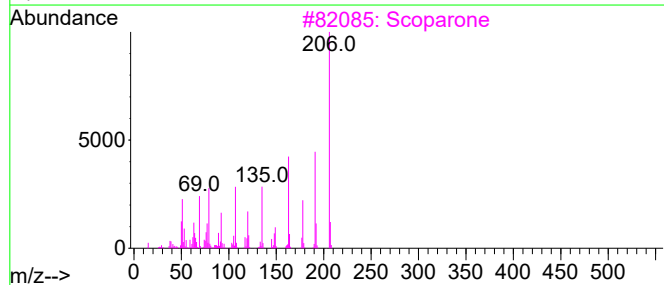
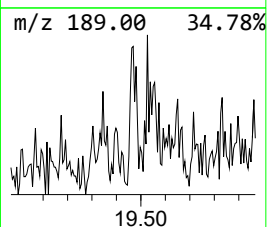
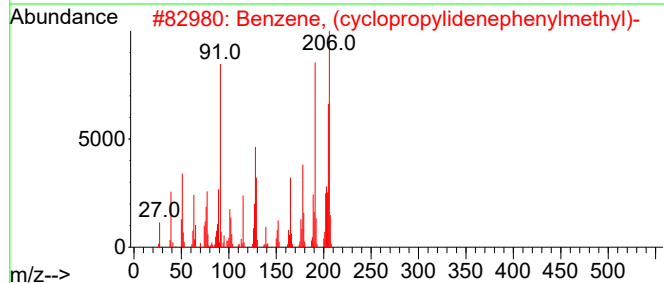
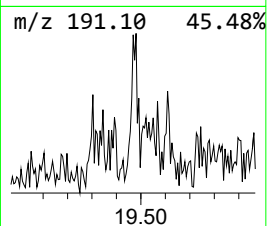
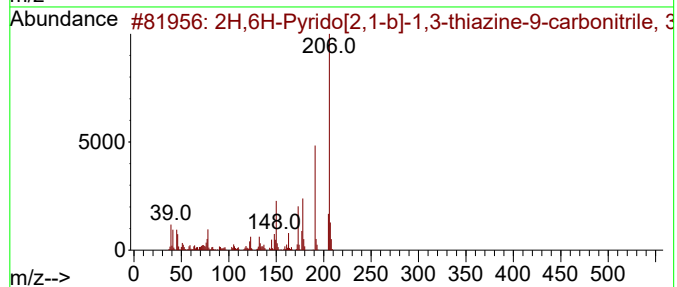
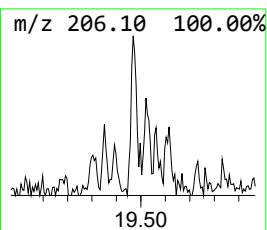
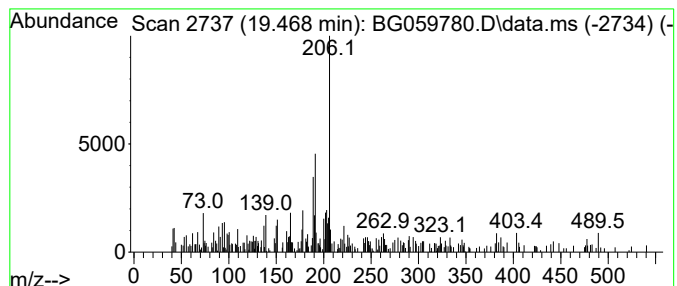
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2H,6H-Pyrido[2,1-b]-1,3-thi... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.468	2.30 ng	78895	Phenanthrene-d10	17.711

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H,6H-Pyrido[2,1-b]-1,3-thiazine...	206	C10H10N2OS	1000277-29-6	76
2			Benzene, (cyclopropylidenepheryl...	206	C16H14	007632-57-7	76
3			Scoparone	206	C11H10O4	000120-08-1	64
4			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	64
5			1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	64



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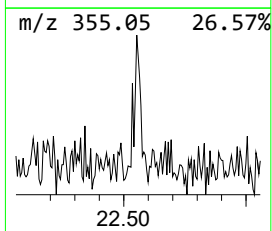
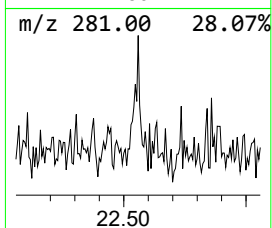
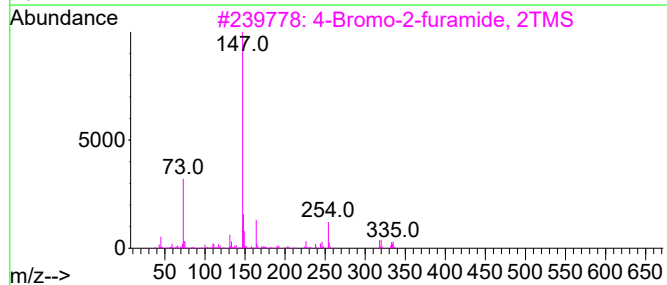
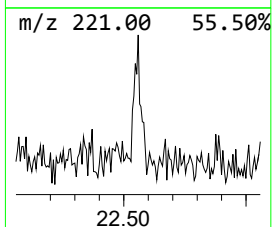
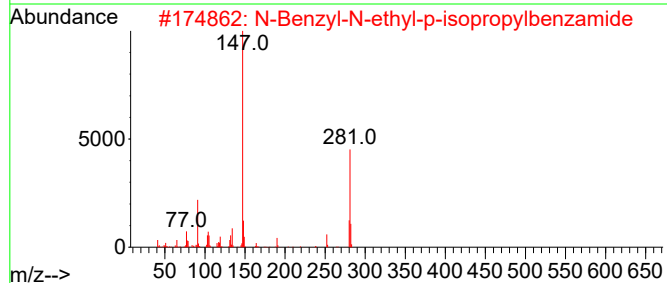
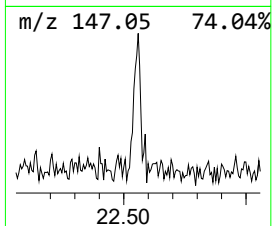
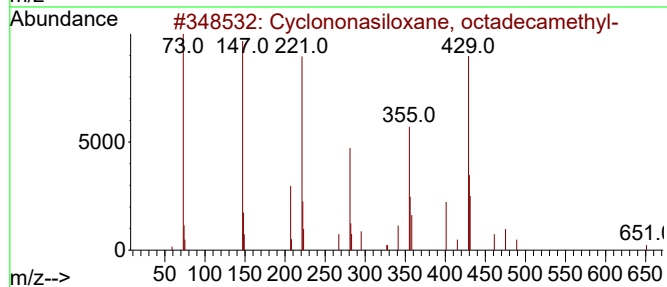
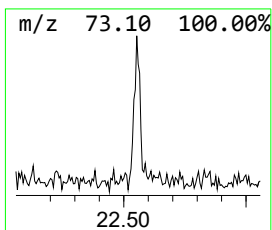
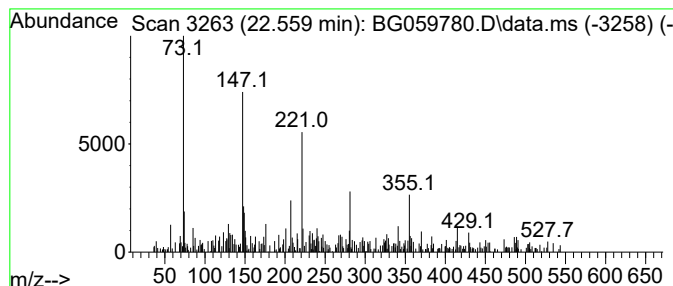
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.559	4.08 ng	129192	Chrysene-d12	22.042

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	50
2		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	43
3		4-Bromo-2-furamide, 2TMS	333	C11H20BrN2O2Si2	1000514-30-2	43
4		5,6-Difluoro-1H-indazole-3-carbo...	342	C14H20F2N2O2Si2	1000500-32-0	38
5		2,4,6-Trimethylbenzoic acid, TMS...	236	C13H20O2Si	070079-88-8	38



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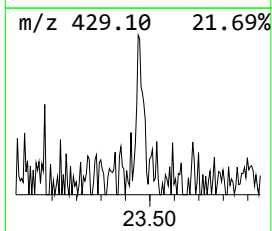
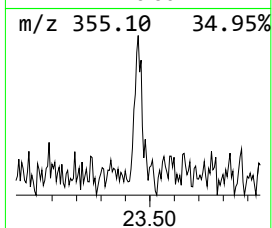
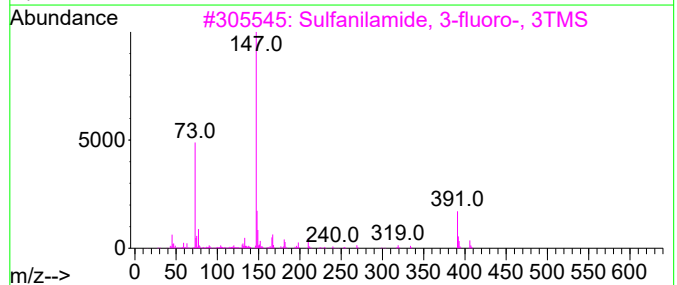
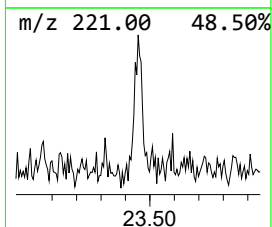
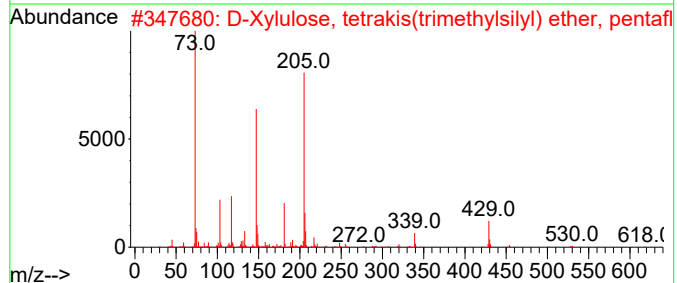
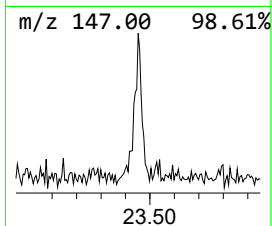
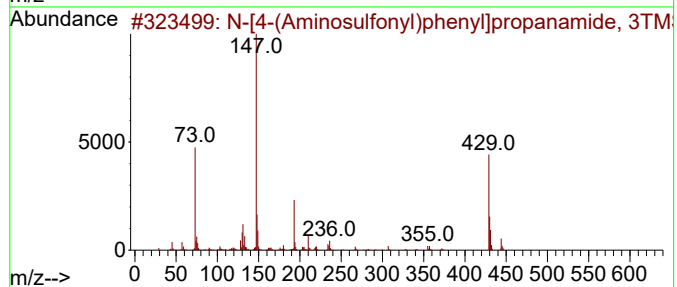
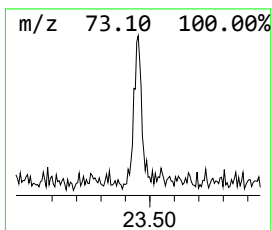
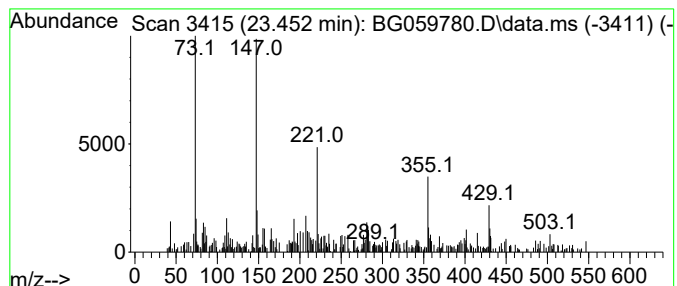
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 N-[4-(Aminosulfonyl)phenyl]... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.452	5.95 ng	188168	Chrysene-d12	22.042

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-[4-(Aminosulfonyl)phenyl]propa...	444	C18H36N2O3SSi3	1000500-82-8	68
2			D-Xylulose, tetrakis(trimethylsi...	633	C24H44F5NO5Si4	1000394-61-4	53
3			Sulfanilamide, 3-fluoro-, 3TMS	406	C15H31FN2O2SSi3	1000509-50-3	45
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	45
5			D-Xylulose, tetrakis(trimethylsi...	633	C24H44F5NO5Si4	1000394-61-3	42



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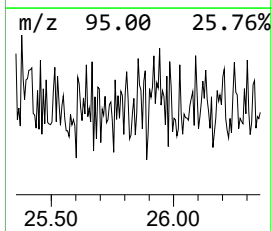
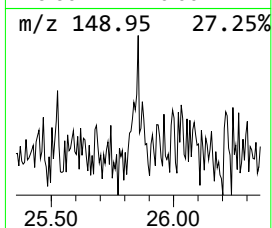
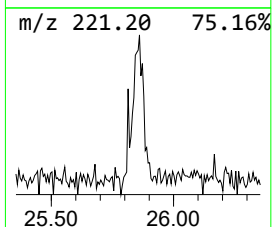
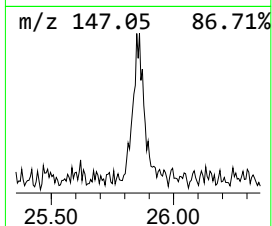
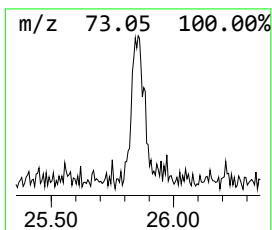
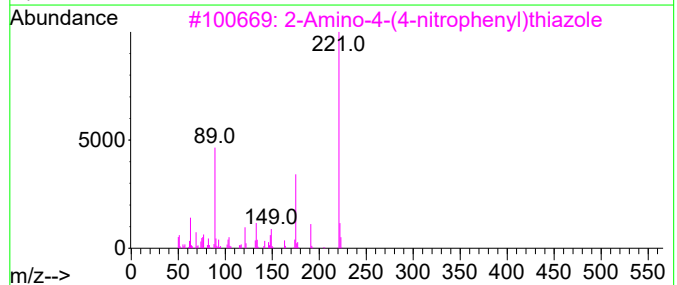
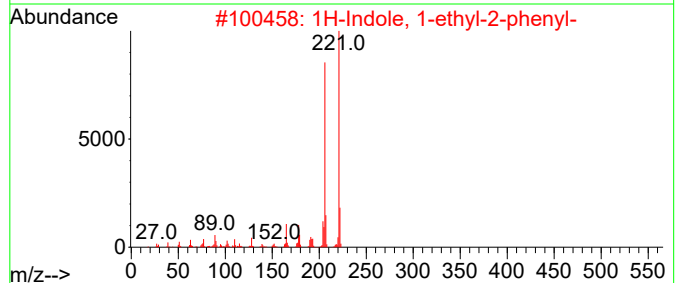
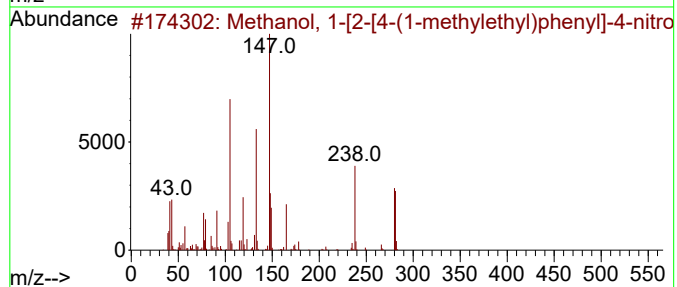
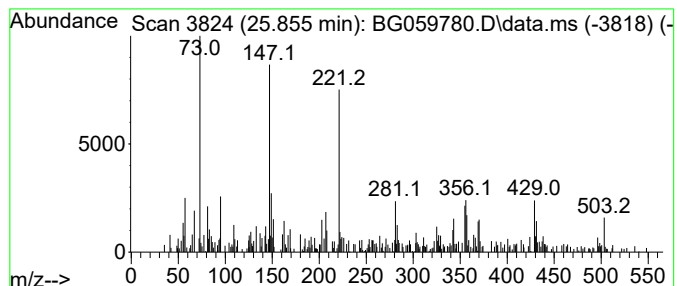
Instrument :
BNA_G
ClientSampleId :
210

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 5 unknown25.855 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.855	20.00 ng	356439	Perylene-d12	25.626	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanol, 1-[2-[4-(1-methylethyl...	281	C14H19NO5	1000271-97-1	22
2	1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	18
3	2-Amino-4-(4-nitrophenyl)thiazole	221	C9H7N3O2S	002104-09-8	18
4	Mono-3-methylbut-3-enyl phthalat...	306	C16H22O4Si	1010373-63-6	14
5	[2-[(4-methoxyphenyl)imino]-4-me...	252	C12H16N2O2S	283170-80-9	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059780.D
Acq On : 20 Nov 2023 22:30
Operator : MA/JU
Sample : 05376-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

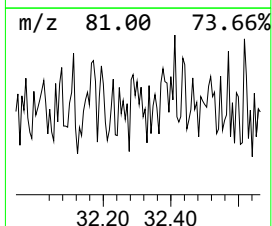
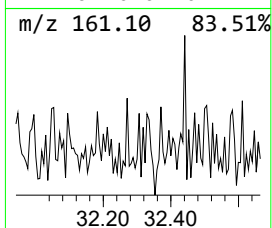
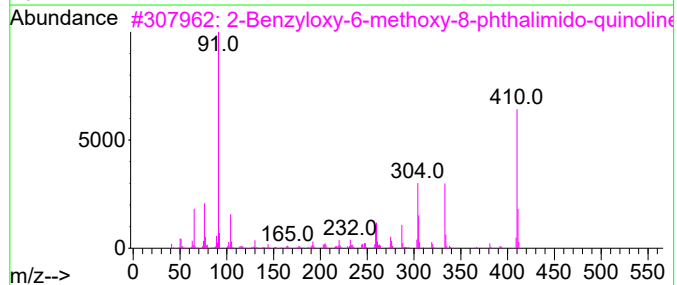
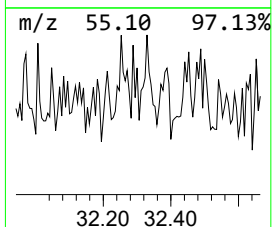
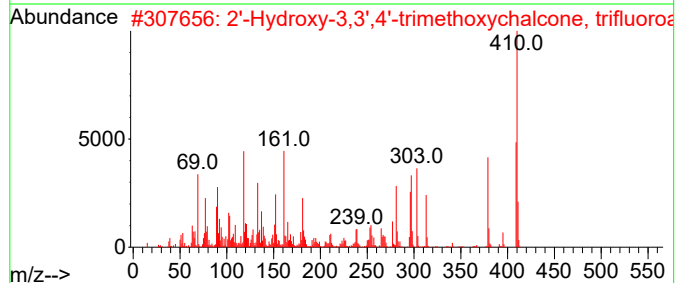
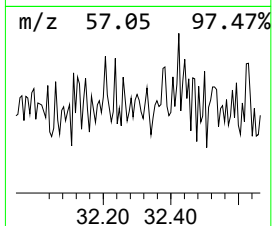
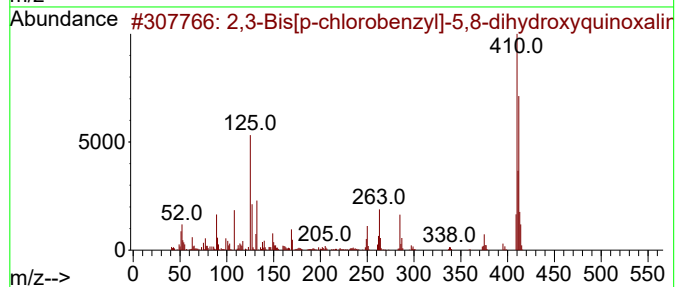
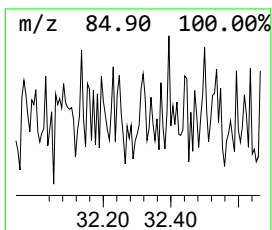
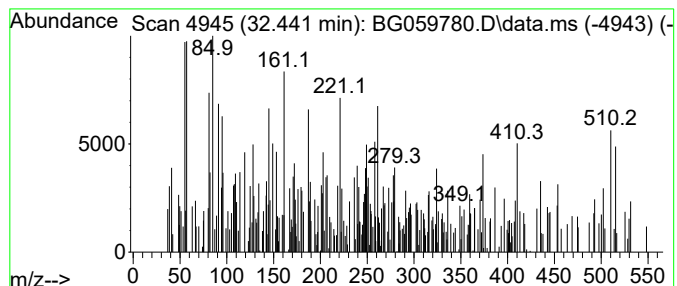
Instrument :
BNA_G
ClientSampleId :
210

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 unknown32.441 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
32.441	2.45 ng	43657	Perylene-d12		25.626	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,3-Bis[p-chlorobenzyl]-5,8-dihy...		410	C22H16Cl2N2O2	056393-54-5	25
2	2'-Hydroxy-3,3',4'-trimethoxycha...		410	C20H17F3O6	1010453-84-8	11
3	2-Benzyloxy-6-methoxy-8-phthalim...		410	C25H18N2O4	1000213-27-2	10
4	3,6-Dibromobenzo[e]pyrene		408	C20H10Br2	077508-03-3	10
5	Ajmaline diacetate		410	C24H30N2O4	019775-56-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
Data File : BG059780.D
Acq On : 20 Nov 2023 22:30
Operator : MA/JU
Sample : 05376-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
210

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
2,4,7,9-Tetrame...	13.793	19.6	ng	566750	3	14.962	577837	20.0
2H,6H-Pyrido[2,...	19.468	2.3	ng	78895	4	17.711	685513	20.0
Cyclononasiloxa...	22.559	4.1	ng	129192	5	22.042	632751	20.0
N-[4-(Aminosulf...	23.452	6.0	ng	188168	5	22.042	632751	20.0
unknown25.855	25.855	20.0	ng	356439	6	25.626	356439	20.0
unknown32.441	32.441	2.5	ng	43657	6	25.626	356439	20.0