

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
 Data File : BF134923.D
 Acq On : 24 Aug 2023 14:36
 Operator : CG\JU
 Sample : 04100-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-1

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_F\Methods\8270-BF082223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134923.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	563	568	571	rBV	2633908	2445218	100.00%	11.005%
2	6.434	734	739	742	rBV	2319423	2327066	95.17%	10.474%
3	6.792	797	800	804	rBV	868772	653390	26.72%	2.941%
4	7.357	891	896	899	rBV	1685731	1489682	60.92%	6.705%
5	8.069	1014	1017	1020	rBV	895105	777254	31.79%	3.498%
6	9.069	1181	1187	1189	rBV3	58673	92271	3.77%	0.415%
7	9.151	1197	1201	1204	rBV	2812514	2371304	96.98%	10.673%
8	9.228	1209	1214	1217	rVV3	67504	122908	5.03%	0.553%
9	9.339	1231	1233	1235	rBV3	57421	57067	2.33%	0.257%
10	9.398	1241	1243	1245	rBV3	56175	54854	2.24%	0.247%
11	9.539	1264	1267	1268	rBV2	102970	109944	4.50%	0.495%
12	9.592	1274	1276	1280	rBV4	126309	176251	7.21%	0.793%
13	9.692	1291	1293	1296	rBV2	241104	278282	11.38%	1.252%
14	9.739	1299	1301	1304	rVB	331196	310488	12.70%	1.397%
15	9.833	1311	1317	1320	rBV2	954640	1251188	51.17%	5.631%
16	9.880	1321	1325	1326	rBV3	226981	344655	14.10%	1.551%
17	10.204	1378	1380	1383	rVB3	386952	370608	15.16%	1.668%
18	10.245	1384	1387	1389	rBV2	497365	509571	20.84%	2.293%
19	10.633	1450	1453	1457	rBV2	1030653	1249418	51.10%	5.623%
20	12.945	1844	1846	1854	rVB	1198991	1277716	52.25%	5.751%
21	13.998	2022	2025	2029	rBV2	824499	1160785	47.47%	5.224%
22	15.045	2199	2203	2206	rBV	810511	1187954	48.58%	5.347%
23	15.151	2218	2221	2224	rVB	213212	228541	9.35%	1.029%
24	15.345	2251	2254	2260	rVB	495308	618337	25.29%	2.783%
25	15.410	2261	2265	2271	rVV	682801	854650	34.95%	3.847%
26	15.474	2272	2276	2279	rVV	533499	714373	29.22%	3.215%
27	15.504	2279	2281	2290	rVB2	232948	322633	13.19%	1.452%
28	16.957	2523	2528	2536	rVB2	251674	518626	21.21%	2.334%
29	17.409	2600	2605	2612	rVB	174673	343443	14.05%	1.546%

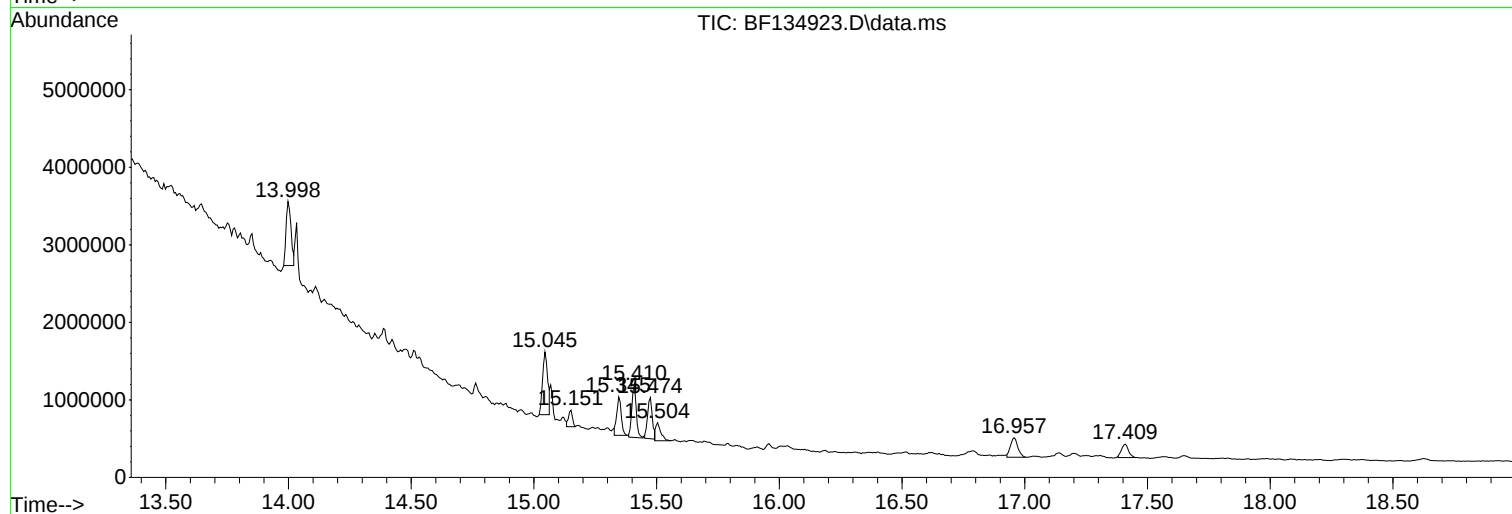
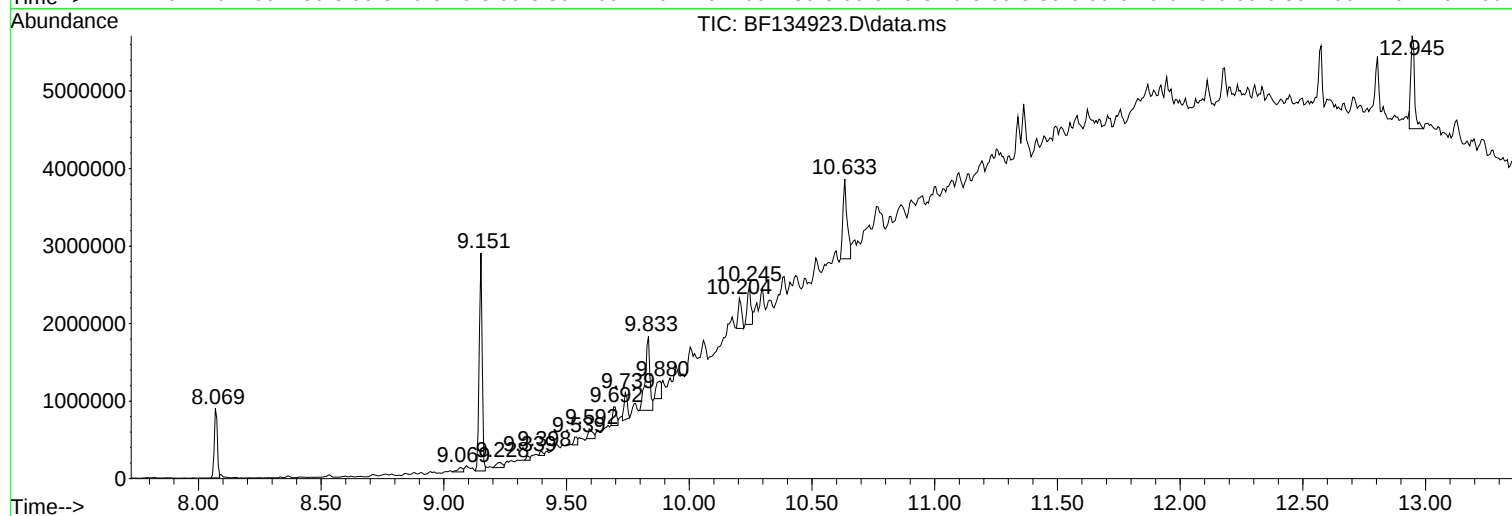
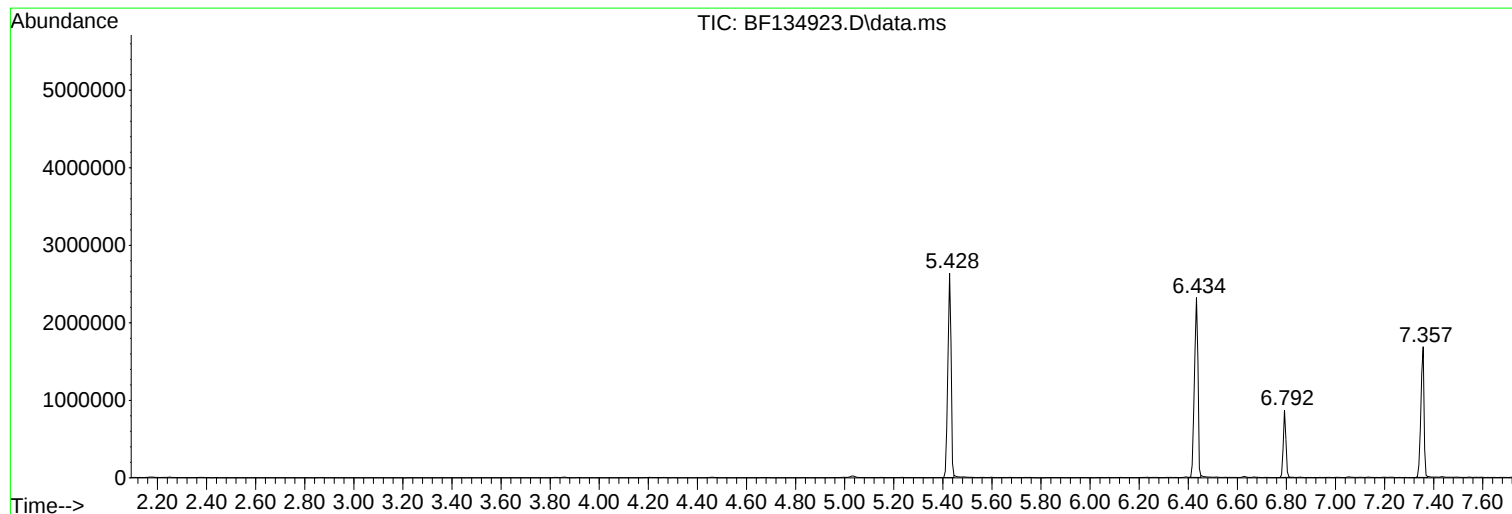
Sum of corrected areas: 22218477

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134923.D
Acq On : 24 Aug 2023 14:36
Operator : CG\JU
Sample : 04100-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134923.D
Acq On : 24 Aug 2023 14:36
Operator : CG\JU
Sample : 04100-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

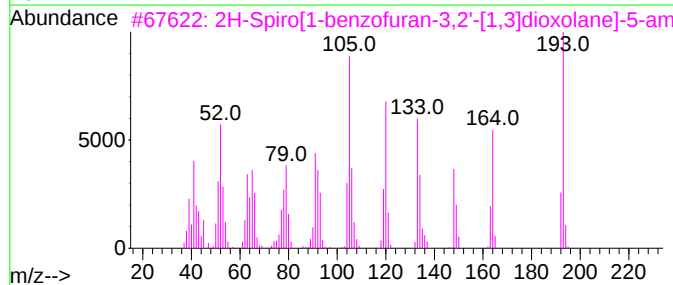
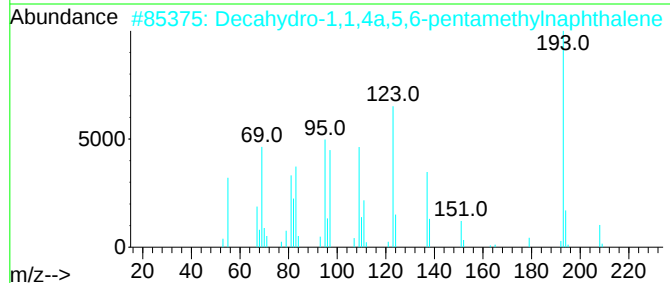
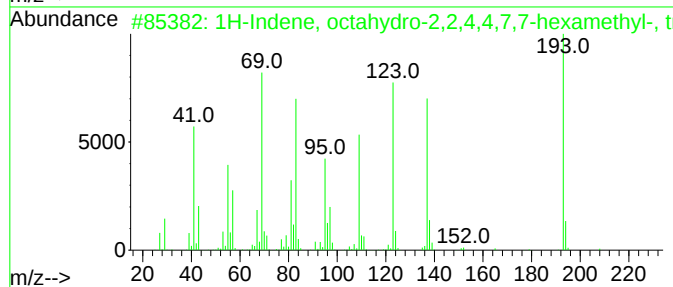
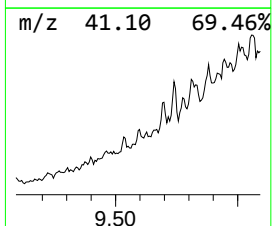
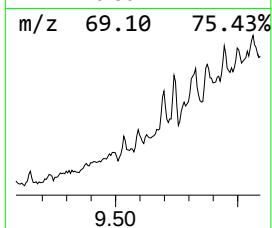
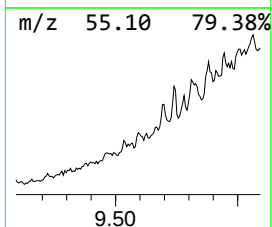
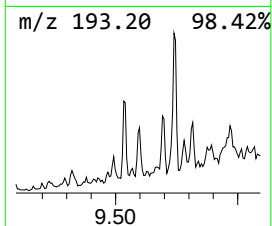
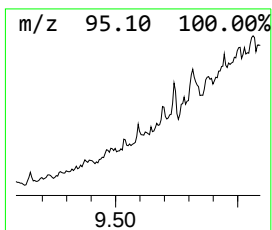
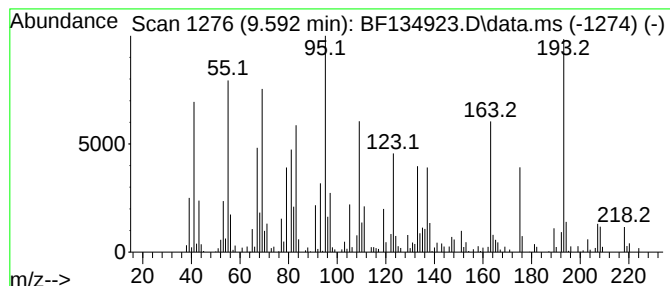
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown9.592 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.592	2.82 ng	176251	Acenaphthene-d10	9.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,7,7...	208	C15H28	054832-83-6	43		
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30		
3	2H-Spiro[1-benzofuran-3,2'-[1,3]...	193	C10H11NO3	1000387-33-4	25		
4	4-[(4-Fluorophenyl)methyl]piperi...	193	C12H16FN	092822-02-1	25		
5	Bicyclo[2.2.1]heptane-2,3-dione,...	166	C10H14O2	010334-26-6	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134923.D
Acq On : 24 Aug 2023 14:36
Operator : CG\JU
Sample : 04100-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

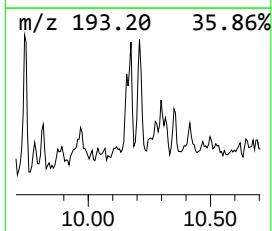
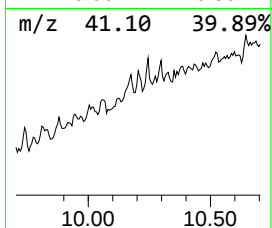
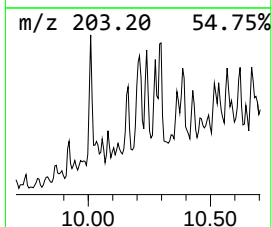
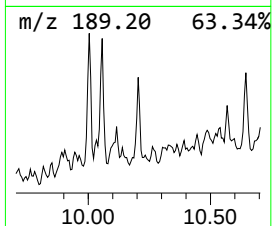
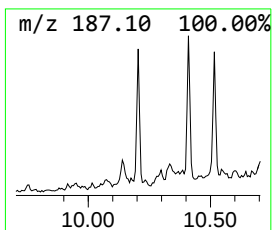
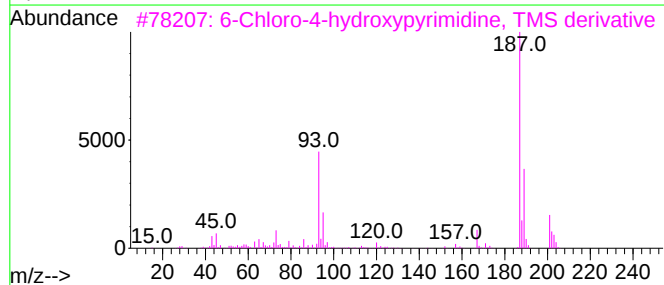
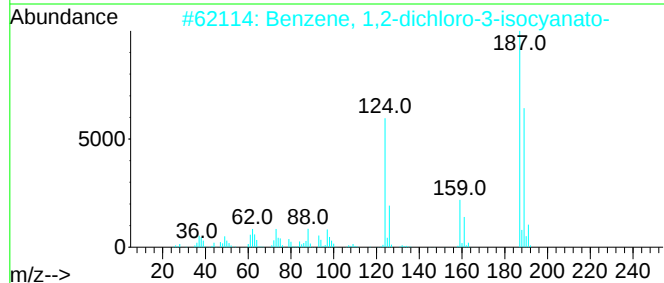
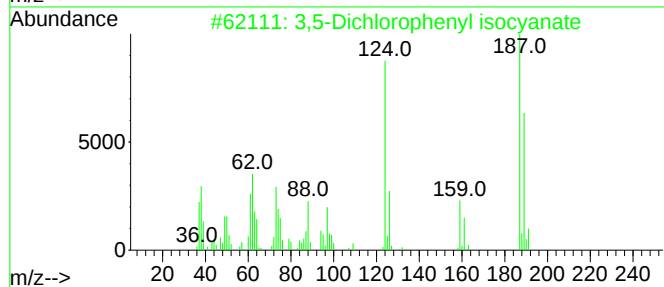
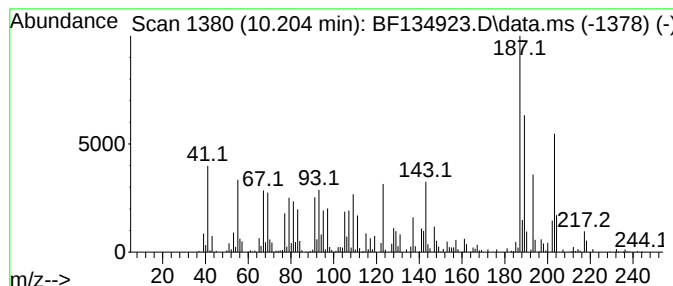
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown10.204 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.204	5.92 ng	370608	Acenaphthene-d10	9.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5-Dichlorophenyl isocyanate	187	C7H3Cl2NO	034893-92-0	38
2			Benzene, 1,2-dichloro-3-isocyanato-	187	C7H3Cl2NO	041195-90-8	38
3			6-Chloro-4-hydroxypyrimidine, TM...	202	C7H11ClN2OSi	1000468-43-3	35
4			Benzene, 1,3-dichloro-2-isocyanato-	187	C7H3Cl2NO	039920-37-1	35
5			2,4-Dichloropyrrolo[3,2-d]pyrimi...	187	C6H3Cl2N3	063200-54-4	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134923.D
Acq On : 24 Aug 2023 14:36
Operator : CG\JU
Sample : 04100-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

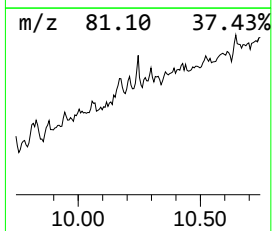
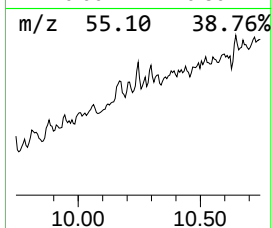
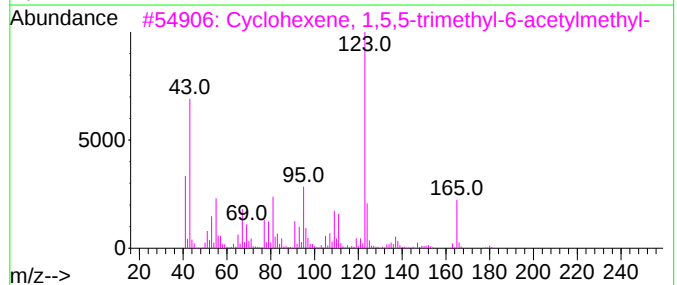
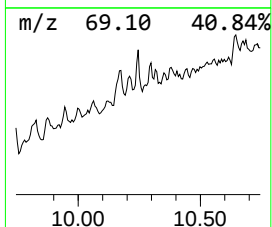
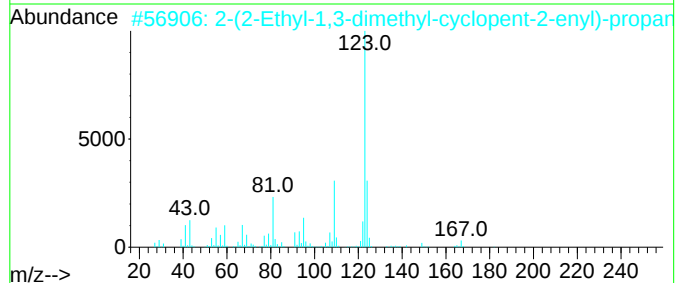
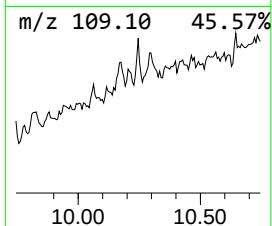
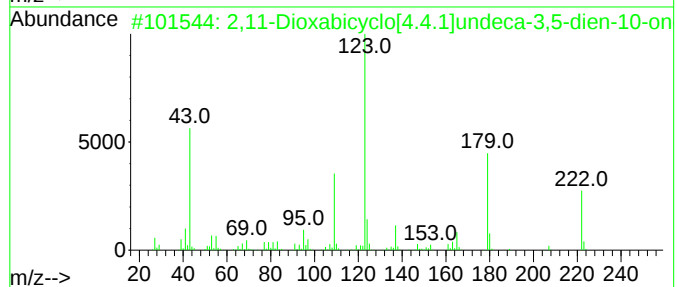
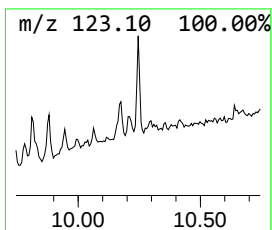
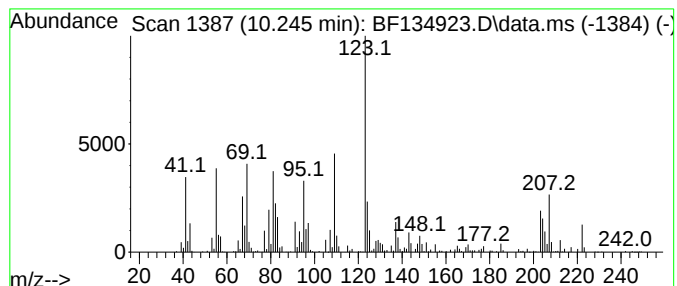
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.245	8.15 ng	509571	Acenaphthene-d10	9.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	50
2			2-(2-Ethyl-1,3-dimethyl-cyclopent...	182	C12H22O	1000186-82-4	47
3			Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	43
4			1H-Purine-2,6-dione, 1,3-diethyl...	222	C10H14N4O2	054965-57-0	43
5			N-[1-(4-Chlorobenzyl)-2-oxoazepa...	374	C20H20ClFN2O2	1000481-70-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134923.D
Acq On : 24 Aug 2023 14:36
Operator : CG\JU
Sample : 04100-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

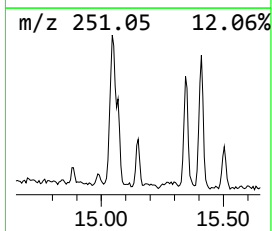
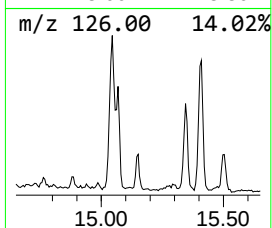
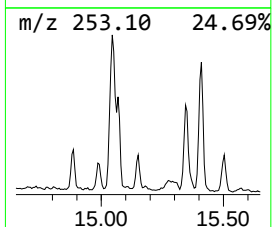
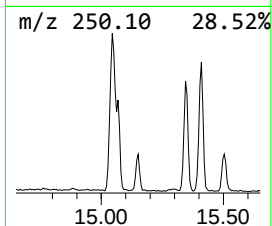
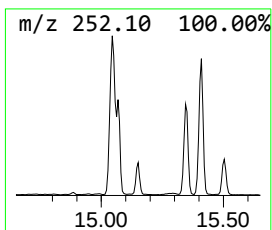
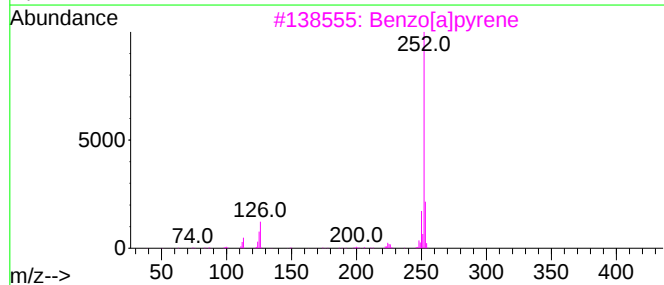
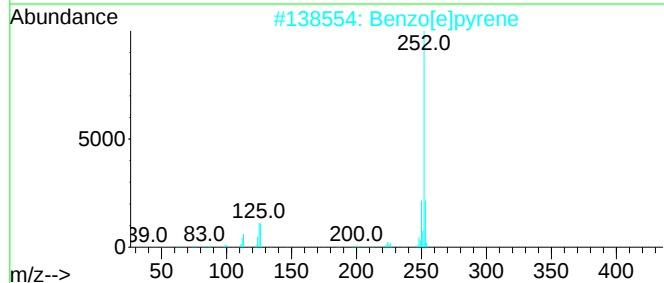
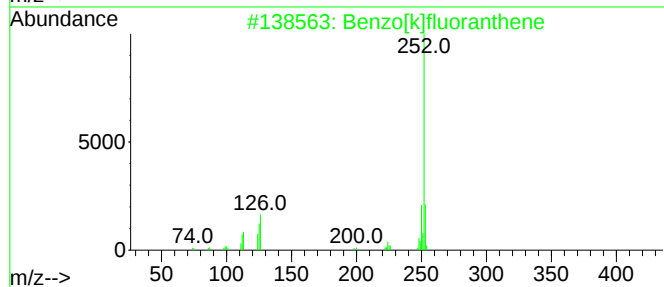
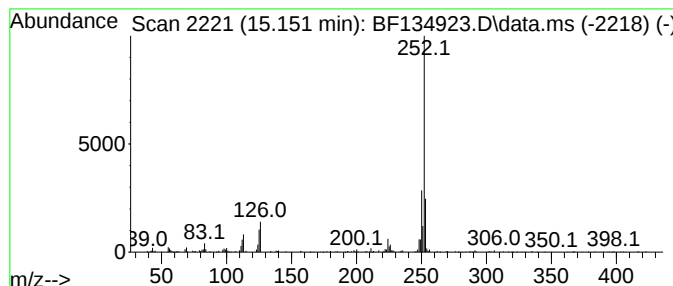
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	6.40 ng	228541	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
2			Benzo[e]pyrene	252	C20H12	000192-97-2	93
3			Benzo[a]pyrene	252	C20H12	000050-32-8	91
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5			Perylene	252	C20H12	000198-55-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134923.D
Acq On : 24 Aug 2023 14:36
Operator : CG\JU
Sample : 04100-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

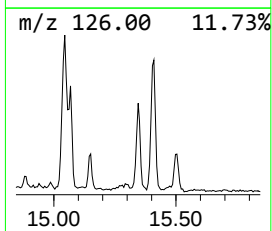
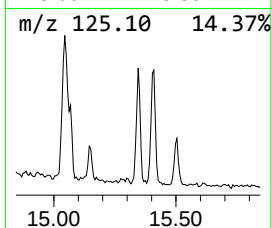
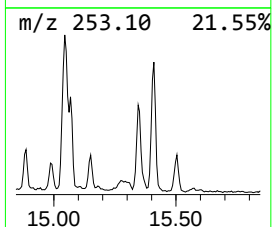
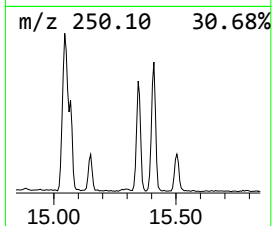
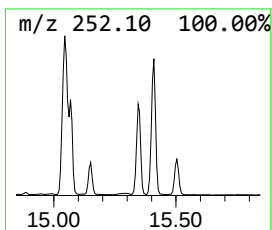
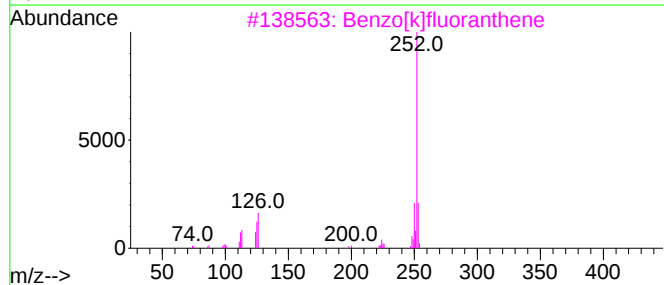
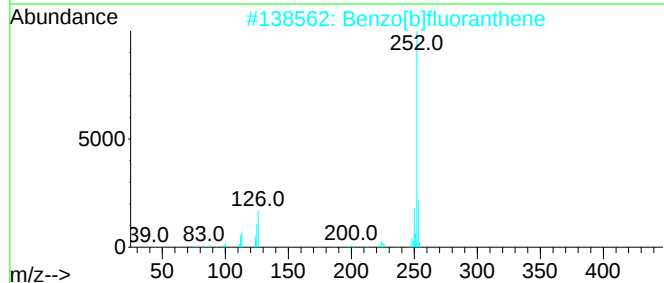
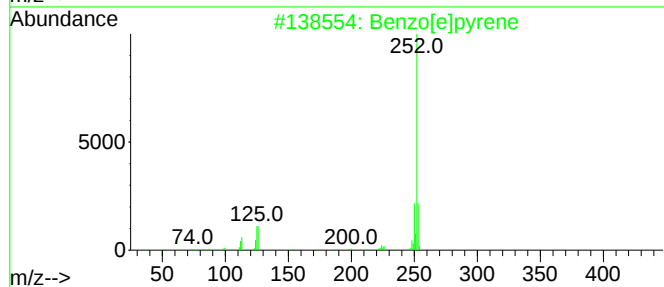
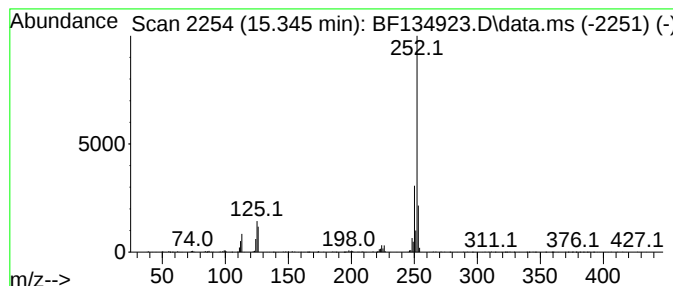
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.345	17.31 ng	618337	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	93
5			Perylene	252	C20H12	000198-55-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134923.D
Acq On : 24 Aug 2023 14:36
Operator : CG\JU
Sample : 04100-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.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
unknown9.592	9.592	2.8	ng	176251	3	9.833	1251190	20.0
unknown10.204	10.204	5.9	ng	370608	3	9.833	1251190	20.0
2,11-Dioxabicyc...	10.245	8.2	ng	509571	3	9.833	1251190	20.0
Benzo[e]pyrene	15.151	6.4	ng	228541	6	15.474	714373	20.0
Perylene	15.345	17.3	ng	618337	6	15.474	714373	20.0