

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
 Data File : BG056283.D
 Acq On : 13 Jan 2023 18:38
 Operator : CG/JU
 Sample : 01135-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-D

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056283.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.331	3	7	16	rVB	159798	222040	7.51%	1.108%
2	5.353	345	351	358	rBV	116288	179750	6.08%	0.897%
3	5.834	426	433	441	rBV	501288	782073	26.47%	3.903%
4	7.450	699	708	722	rBV	512875	874929	29.61%	4.366%
5	8.320	849	856	864	rVB	124030	212752	7.20%	1.062%
6	9.489	1047	1055	1063	rBV	279562	504745	17.08%	2.519%
7	11.152	1330	1338	1345	rBV	171611	312090	10.56%	1.557%
8	13.555	1740	1747	1757	rBV	1143279	1738379	58.83%	8.675%
9	14.930	1969	1981	1987	rBV	363654	559738	18.94%	2.793%
10	14.994	1987	1992	1997	rVB2	21618	34452	1.17%	0.172%
11	16.269	2202	2209	2215	rVB	270692	408527	13.83%	2.039%
12	16.404	2226	2232	2245	rBV	884503	1408914	47.68%	7.031%
13	17.668	2440	2447	2451	rBV	506852	781020	26.43%	3.898%
14	17.709	2451	2454	2460	rVB	131112	178077	6.03%	0.889%
15	17.797	2460	2469	2476	rBV	70662	134463	4.55%	0.671%
16	18.514	2585	2591	2598	rBV3	77708	151869	5.14%	0.758%
17	18.584	2598	2603	2608	rVB2	34931	60775	2.06%	0.303%
18	18.660	2610	2616	2620	rVB	19471	33197	1.12%	0.166%
19	18.731	2620	2628	2632	rBV2	84164	153806	5.21%	0.768%
20	19.019	2672	2677	2682	rBV	32018	48288	1.63%	0.241%
21	19.430	2742	2747	2752	rBV	31905	53254	1.80%	0.266%
22	19.495	2753	2758	2766	rVB8	17182	44946	1.52%	0.224%
23	19.700	2786	2793	2799	rBV	591019	847476	28.68%	4.229%
24	19.941	2827	2834	2842	rBV3	21178	44222	1.50%	0.221%
25	20.024	2842	2848	2850	rVV2	90927	154276	5.22%	0.770%
26	20.059	2850	2854	2860	rVV	491396	715329	24.21%	3.570%
27	20.123	2861	2865	2870	rVB2	23716	35725	1.21%	0.178%
28	20.241	2879	2885	2891	rBV	2362578	2954680	100.00%	14.745%
29	20.370	2902	2907	2914	rBV3	38421	90364	3.06%	0.451%
30	20.541	2924	2936	2941	rVB	116414	229428	7.76%	1.145%
31	20.640	2948	2953	2957	rBV	103897	145079	4.91%	0.724%
32	20.699	2957	2963	2966	rVB4	40257	73269	2.48%	0.366%
33	20.840	2984	2987	2992	rBV	30322	45711	1.55%	0.228%
34	20.887	2992	2995	2999	rVB2	23150	32217	1.09%	0.161%
35	21.328	3066	3070	3075	rVB4	19519	36120	1.22%	0.180%
36	21.545	3095	3107	3115	rBV4	114410	356859	12.08%	1.781%

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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

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.616	3115	3119	3121	rBV2	30033	40371	1.37%	0.201%
38	21.957	3167	3177	3182	rBV3	548553	1404880	47.55%	7.011%
39	22.009	3182	3186	3193	rVB	237890	407648	13.80%	2.034%
40	22.168	3209	3213	3218	rBV	51678	86588	2.93%	0.432%
41	22.391	3245	3251	3258	rBV3	34797	74161	2.51%	0.370%
42	22.726	3305	3308	3313	rVB2	31488	58398	1.98%	0.291%
43	22.803	3318	3321	3329	rVB3	32165	65141	2.20%	0.325%
44	23.167	3379	3383	3390	rVB6	20325	45815	1.55%	0.229%
45	23.708	3473	3475	3484	rVB4	29505	56226	1.90%	0.281%
46	24.307	3567	3577	3584	rBV	180879	636454	21.54%	3.176%
47	24.577	3617	3623	3632	rVB2	39622	104581	3.54%	0.522%
48	25.082	3701	3709	3718	rVB	107835	305739	10.35%	1.526%
49	25.241	3727	3736	3751	rVB	169854	501593	16.98%	2.503%
50	25.406	3754	3764	3773	rBV2	301496	913285	30.91%	4.558%
51	29.360	4428	4437	4458	rVB3	80592	420502	14.23%	2.098%
52	30.611	4638	4650	4663	rVB3	59219	278674	9.43%	1.391%

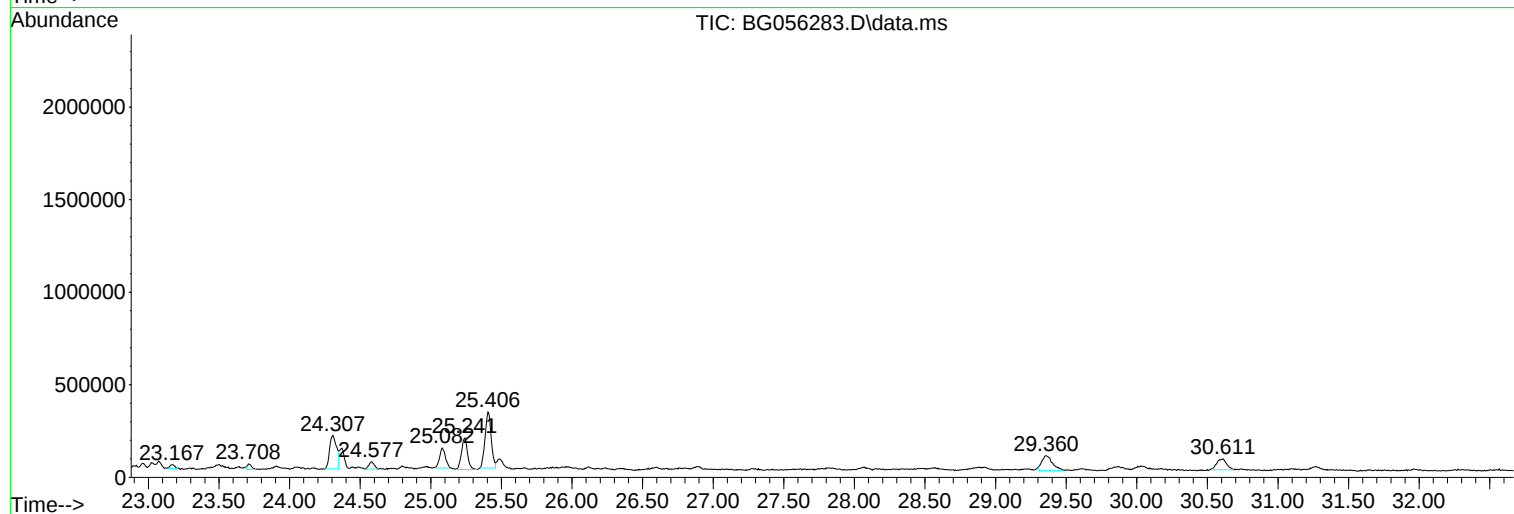
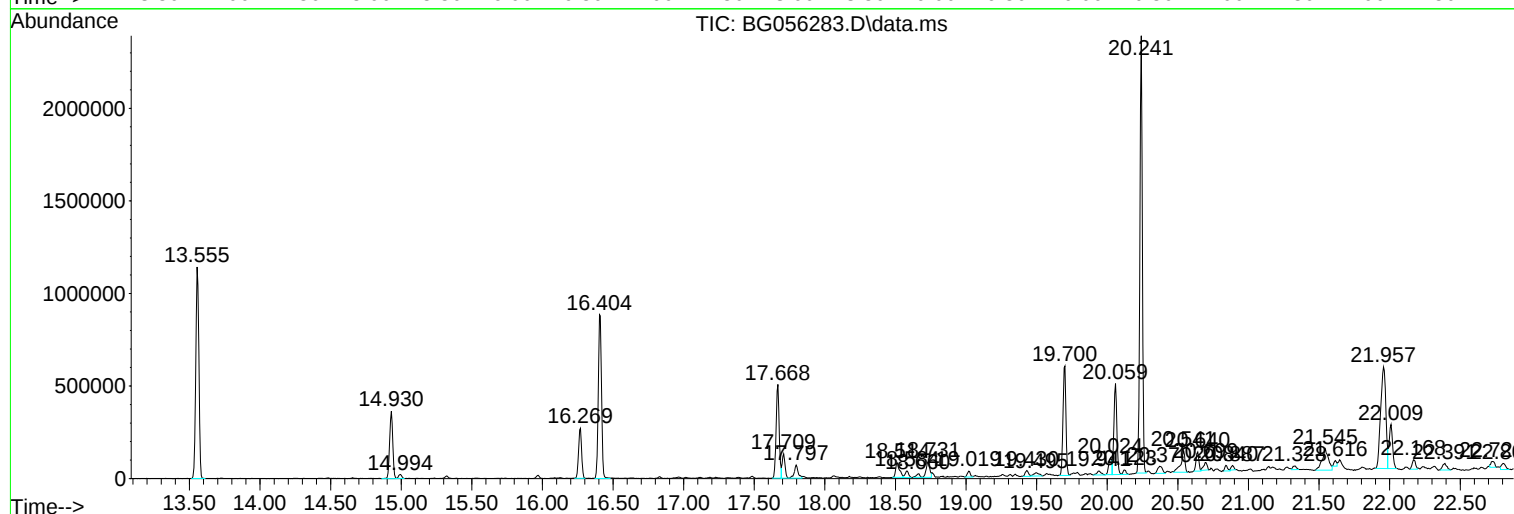
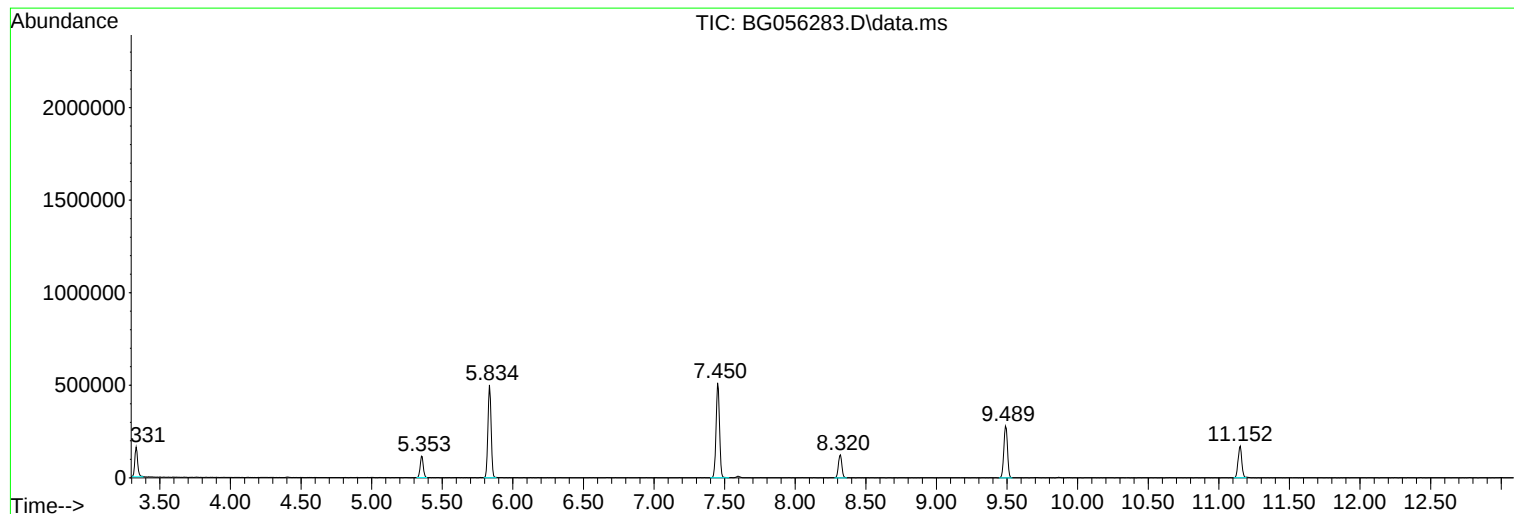
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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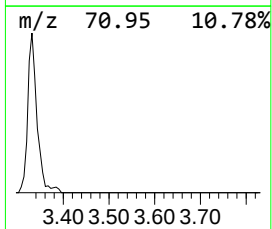
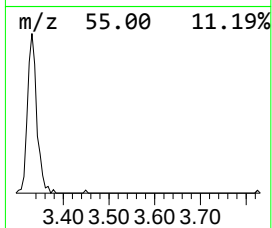
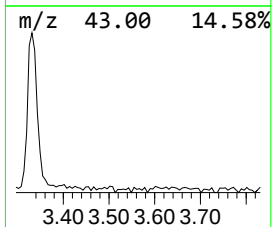
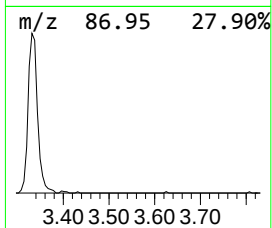
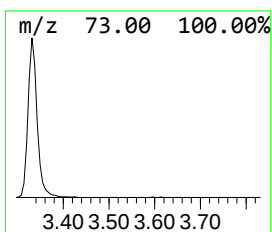
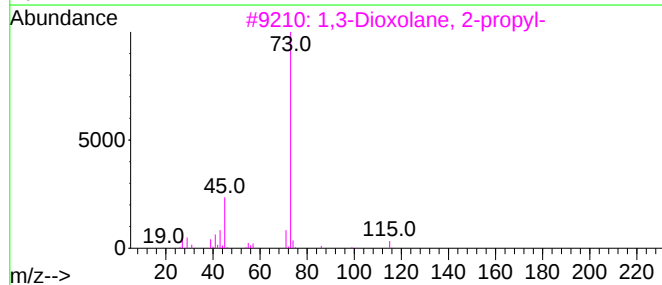
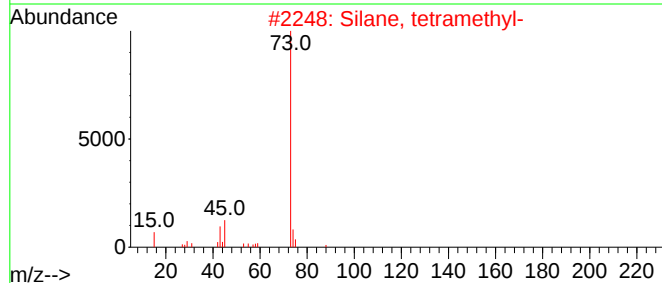
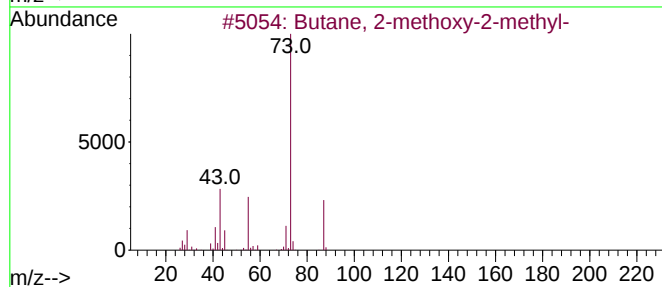
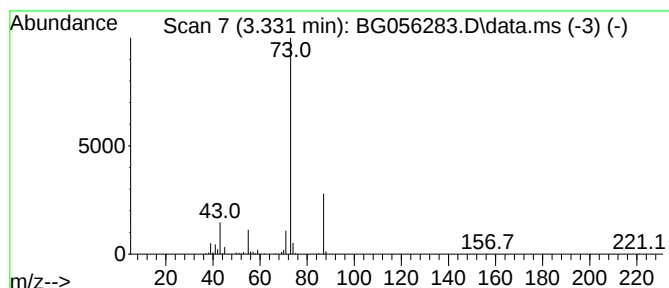
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.331	20.87 ng	222040	1,4-Dichlorobenzene-d4	8.320

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7
5			N-Ethylformamide	73	C3H7NO	000627-45-2	7



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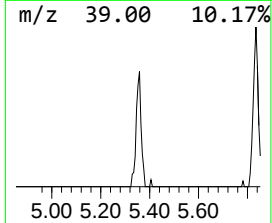
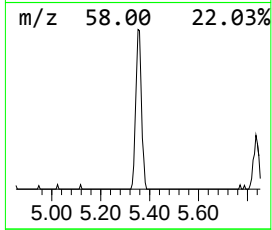
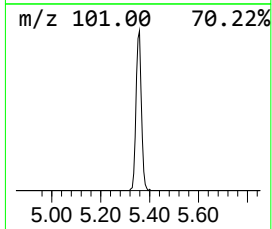
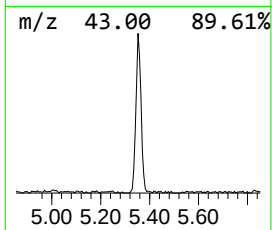
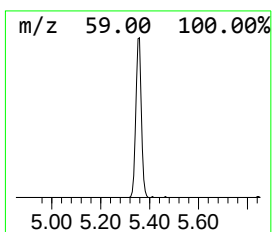
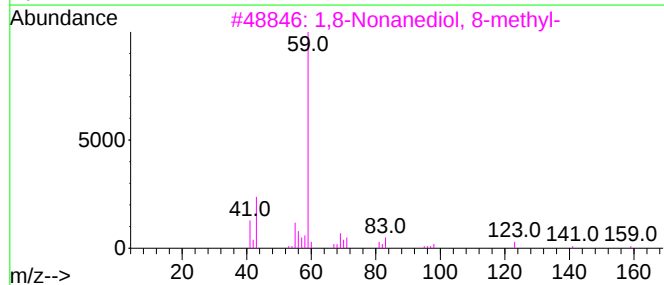
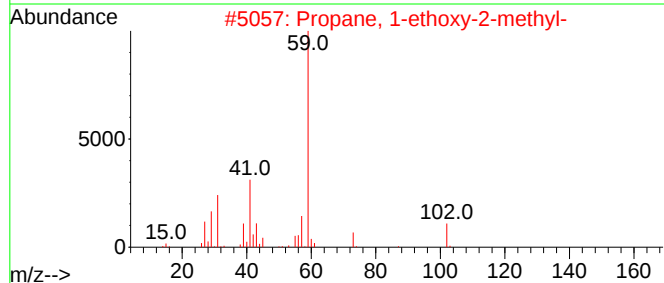
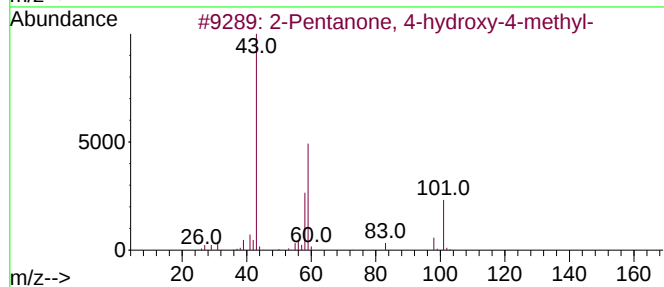
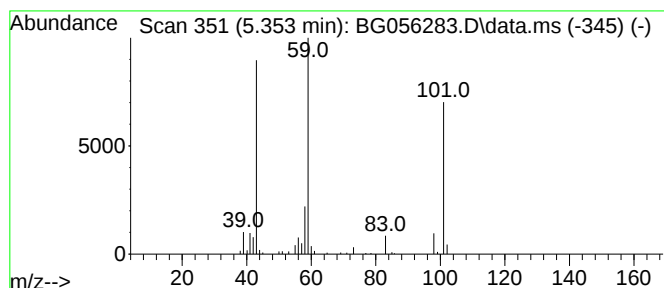
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.353	16.90 ng	179750	1,4-Dichlorobenzene-d4	8.320

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	17



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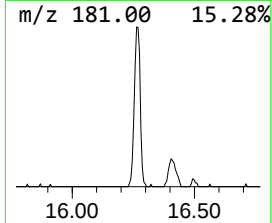
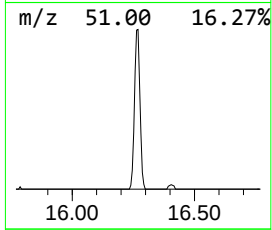
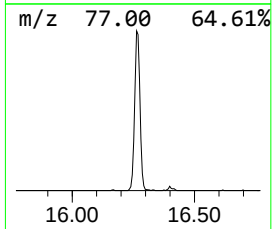
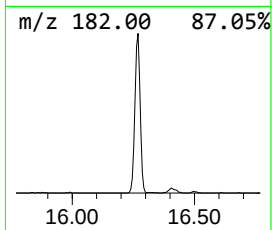
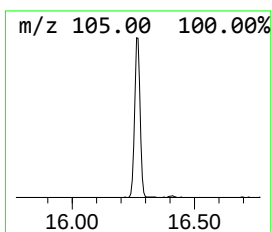
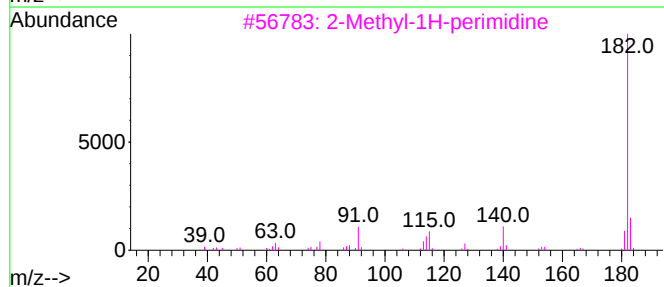
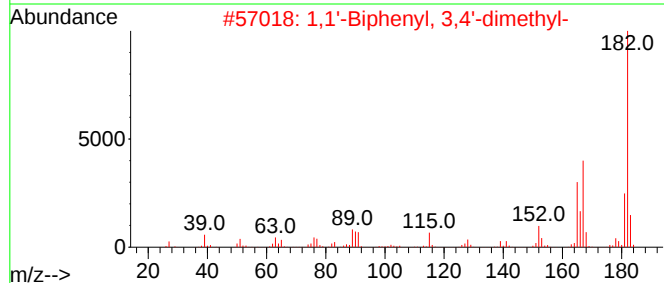
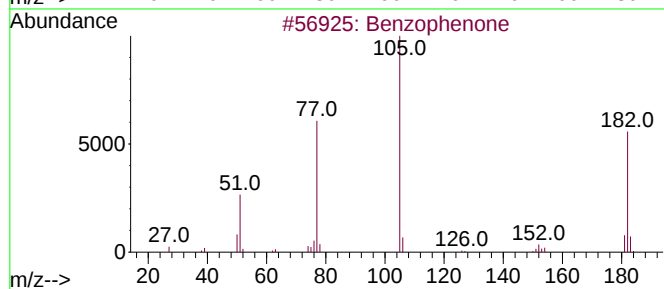
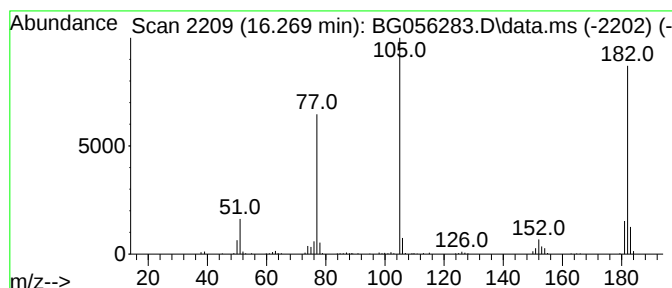
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.269	14.60 ng	408527	Acenaphthene-d10	14.930

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	94
2			1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	52
3			2-Methyl-1H-perimidine	182	C12H10N2	005157-10-8	43
4			Benzilamide	227	C14H13NO2	004746-87-6	35
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	30



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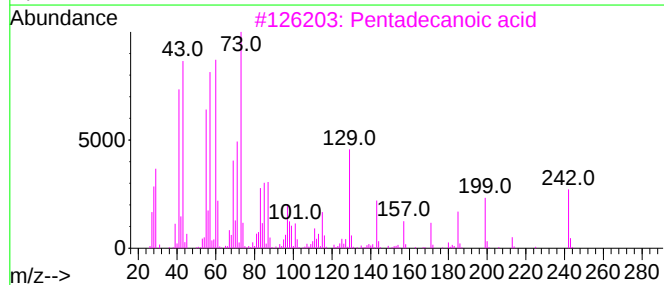
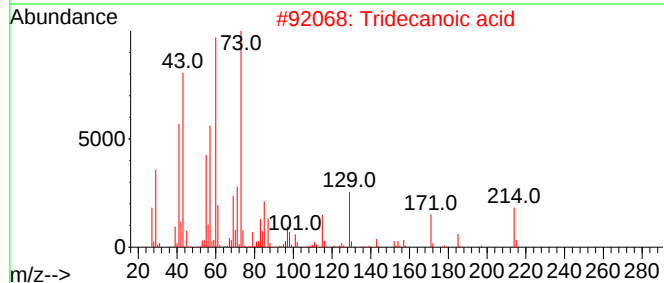
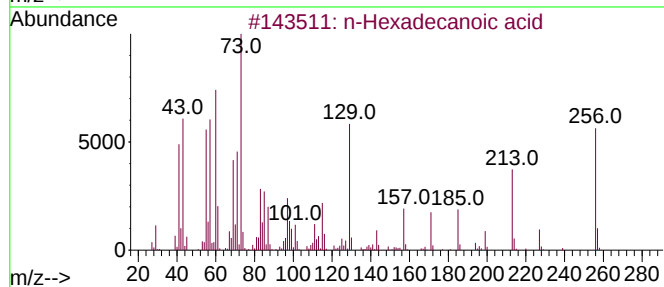
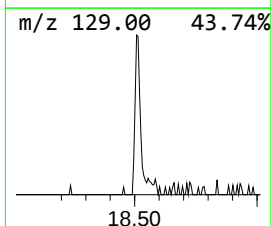
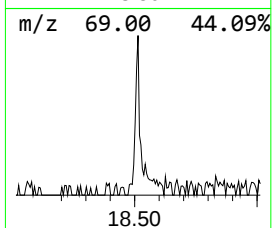
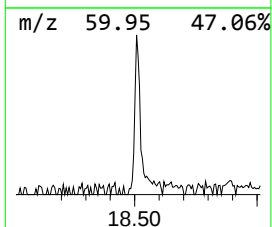
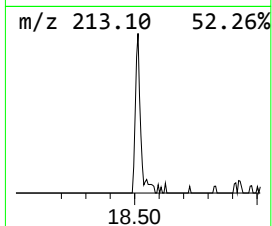
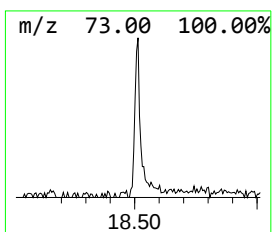
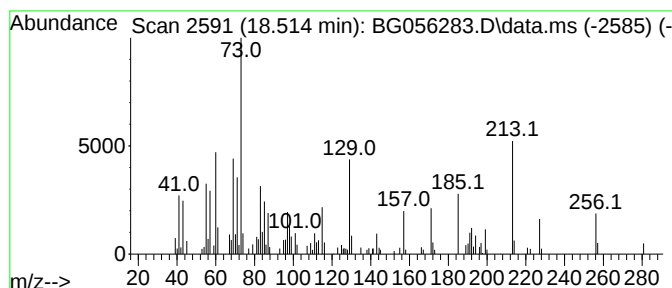
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.514	3.89 ng	151869	Phenanthrene-d10	17.668

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	47
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	38
5		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	32



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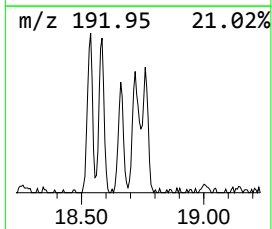
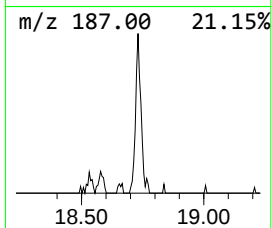
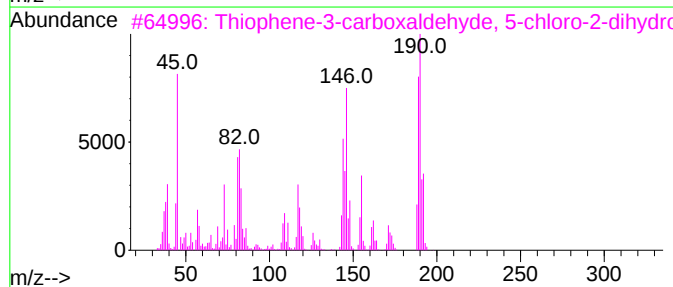
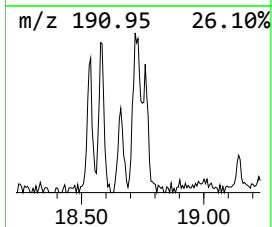
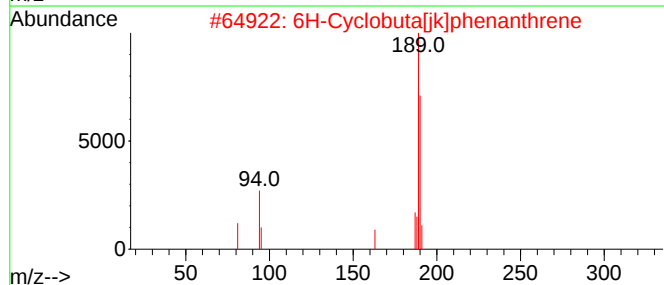
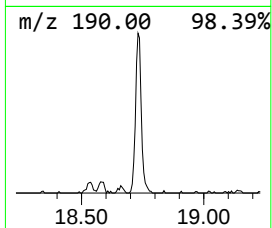
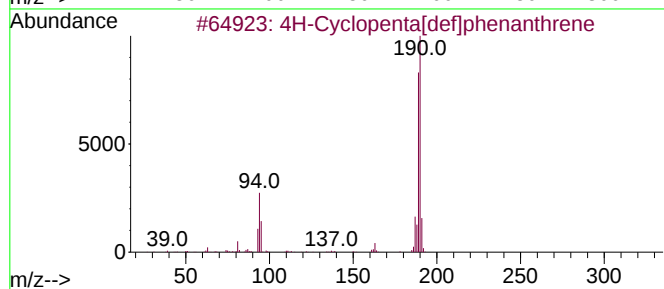
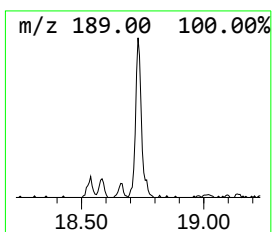
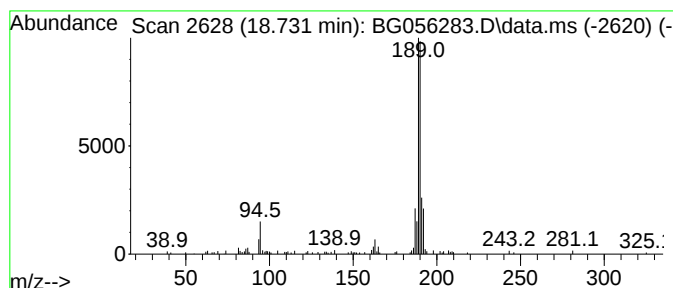
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.731	3.94 ng	153806	Phenanthrene-d10	17.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	59
4			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
5			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056283.D
Acq On : 13 Jan 2023 18:38
Operator : CG/JU
Sample : 01135-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-D

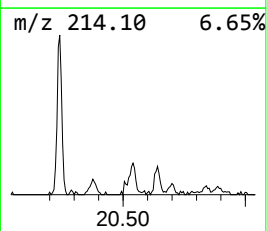
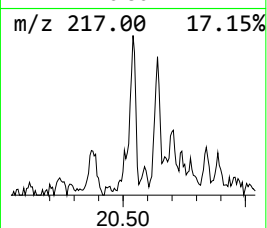
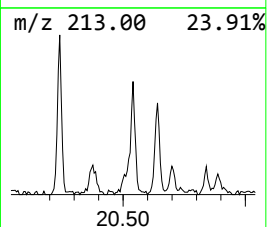
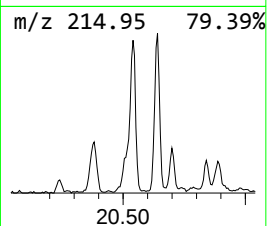
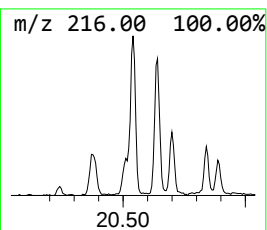
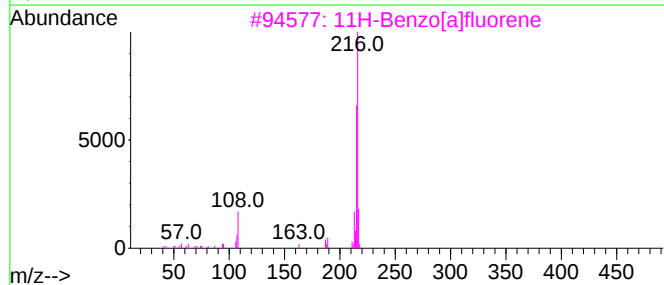
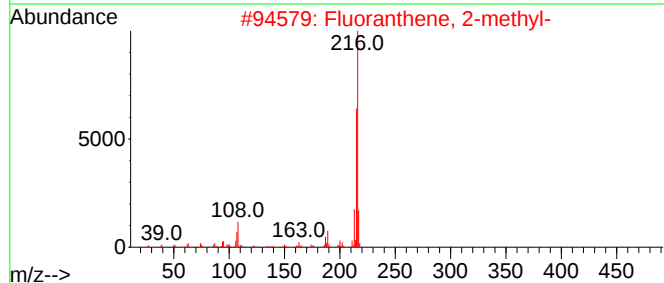
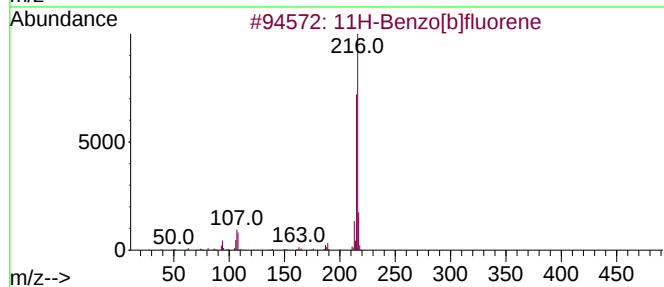
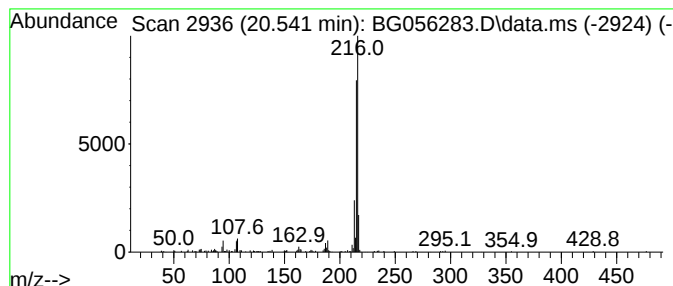
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.541	3.27 ng	229428	Chrysene-d12	21.962

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4		Pyrene, 2-methyl-	216	C17H12	003442-78-2	83
5		Pyrene, 1-methyl-	216	C17H12	002381-21-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056283.D
Acq On : 13 Jan 2023 18:38
Operator : CG/JU
Sample : 01135-04
Misc :
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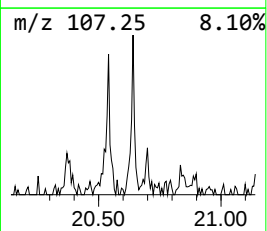
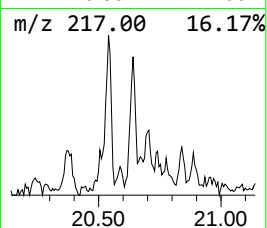
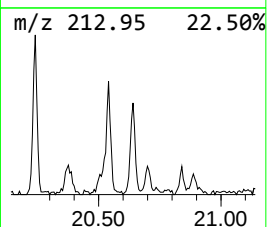
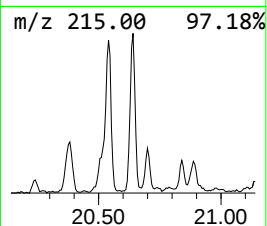
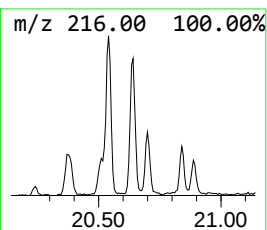
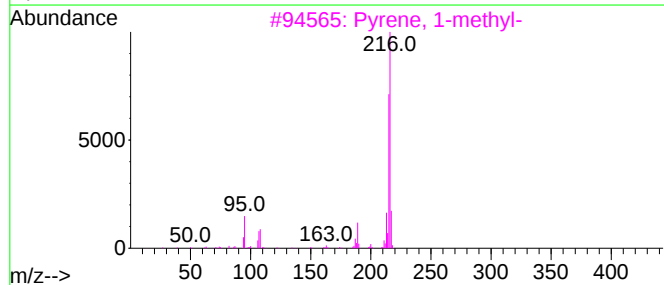
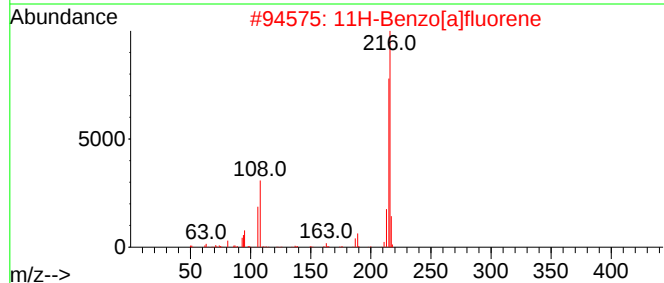
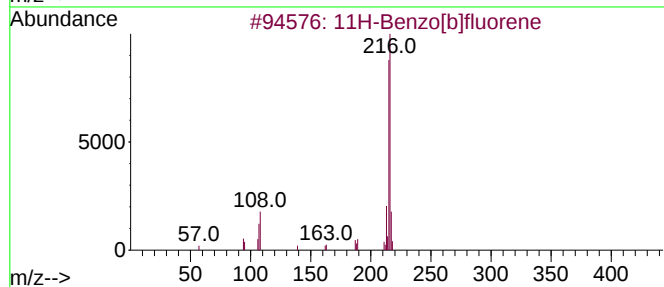
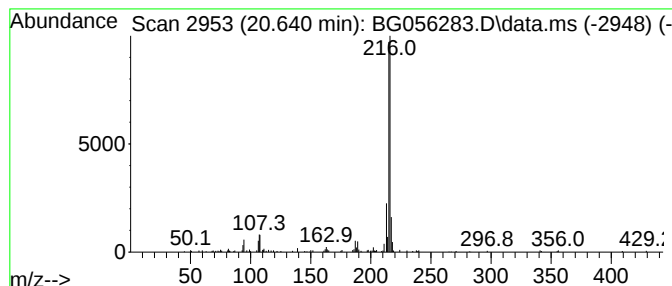
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BNA_G
ClientSampleId :
TP-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11H-Benzo[a]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.640	2.07 ng	145079	Chrysene-d12	21.962	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	70
4	trans-p-(Trifluoromethyl)cinnami...	216	C10H7F3O2	016642-92-5	64
5	1,3,5-Triazine-2,4,6-triamine, N...	216	C10H12N6	046731-79-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056283.D
Acq On : 13 Jan 2023 18:38
Operator : CG/JU
Sample : 01135-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-D

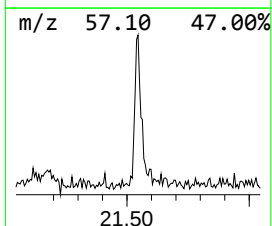
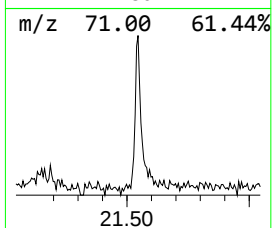
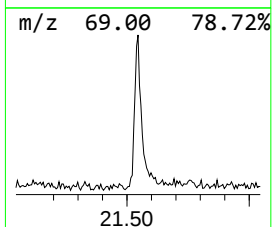
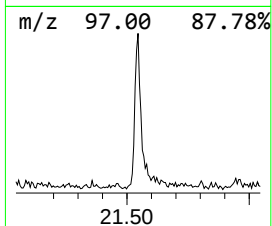
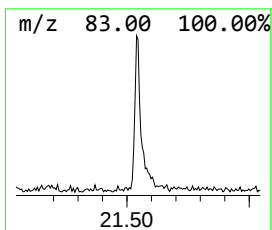
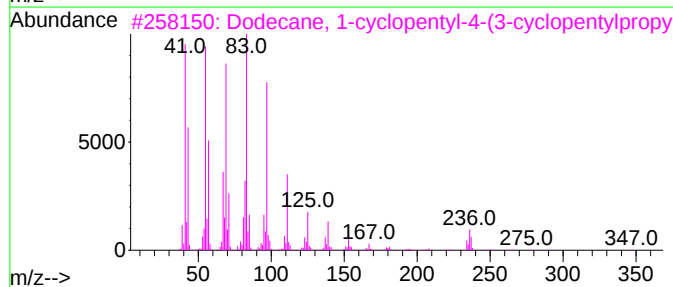
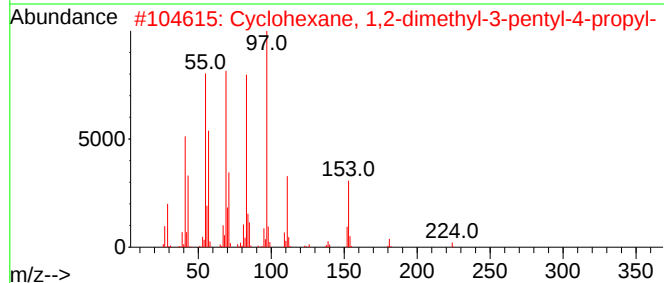
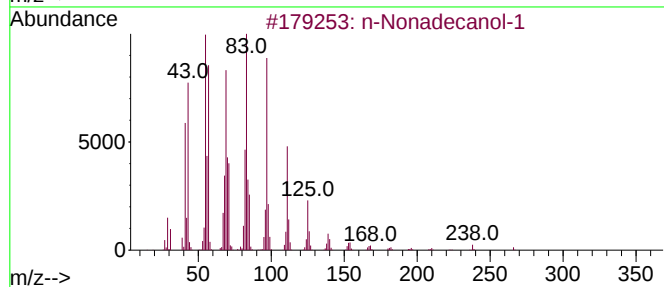
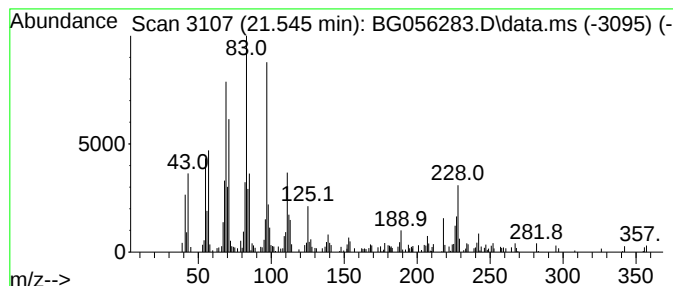
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.545	5.08 ng	356859	Chrysene-d12	21.962

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	80
2		Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	64
3		Dodecane, 1-cyclopentyl-4-(3-cyc...	348	C25H48	007225-68-5	59
4		3-Octadecene, (E)-	252	C18H36	007206-19-1	58
5		Tetracosan-10-ol	354	C24H50O	138966-95-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056283.D
Acq On : 13 Jan 2023 18:38
Operator : CG/JU
Sample : 01135-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-D

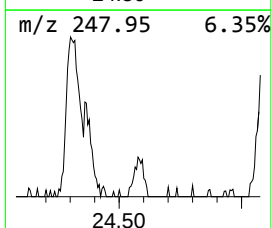
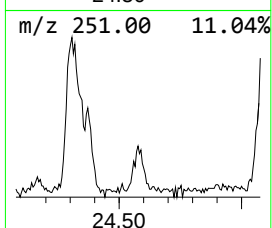
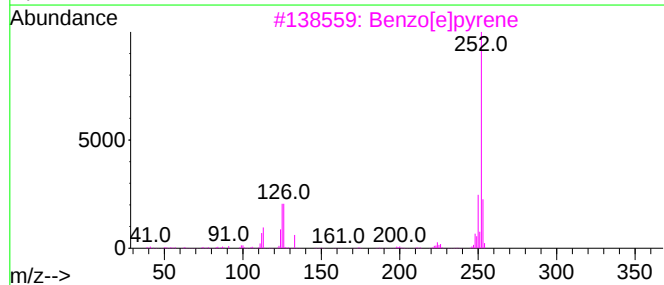
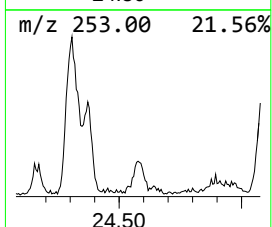
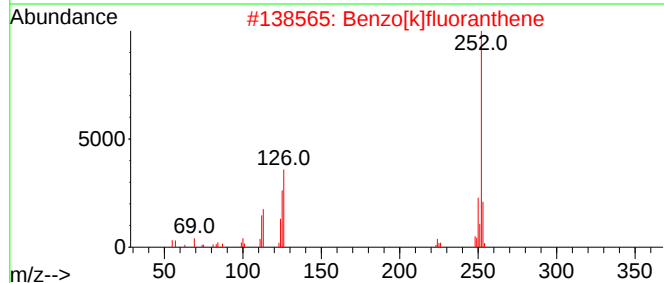
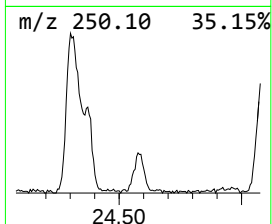
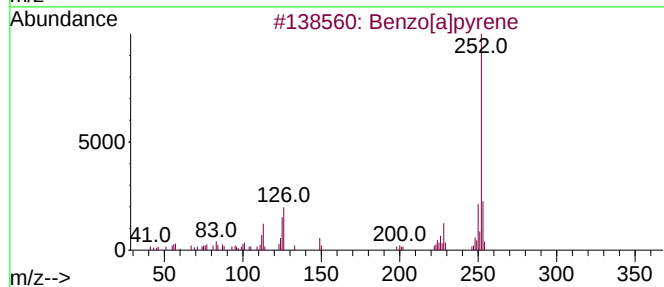
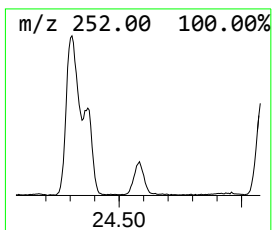
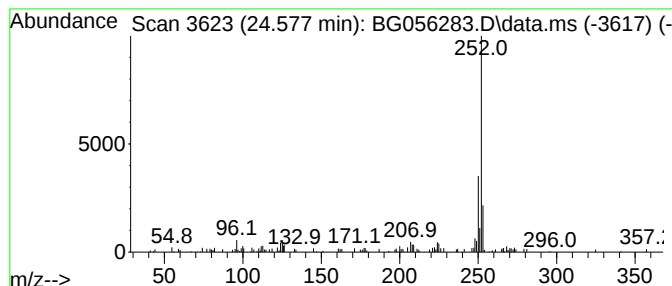
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.577	2.29 ng	104581	Perylene-d12	25.406

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	89
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
3			Benzo[e]pyrene	252	C20H12	000192-97-2	76
4			Perylene	252	C20H12	000198-55-0	76
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056283.D
Acq On : 13 Jan 2023 18:38
Operator : CG/JU
Sample : 01135-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-D

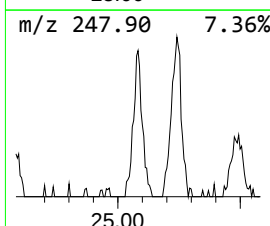
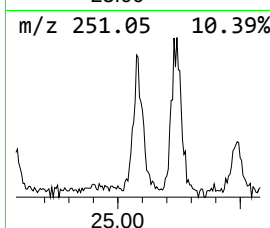
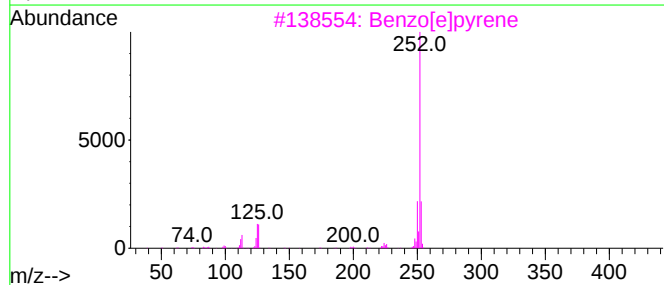
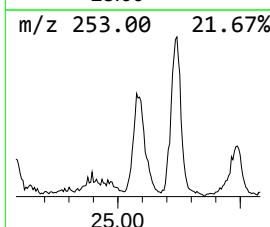
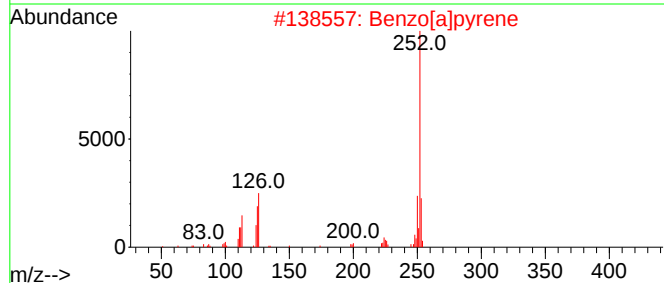
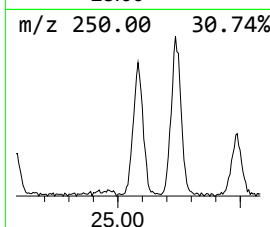
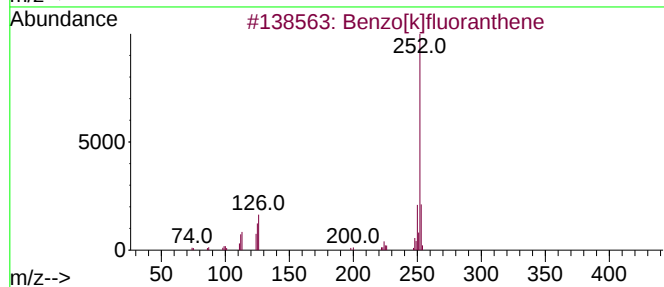
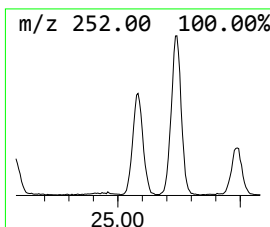
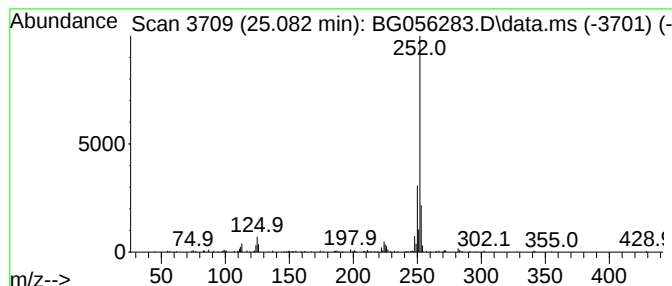
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.082	6.70 ng	305739	Perylene-d12	25.406

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
2		Benzo[a]pyrene	252	C20H12	000050-32-8	90
3		Benzo[e]pyrene	252	C20H12	000192-97-2	81
4		Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
5		Perylene	252	C20H12	000198-55-0	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056283.D
Acq On : 13 Jan 2023 18:38
Operator : CG/JU
Sample : 01135-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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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2-Pentanone, 4-...	5.353	16.9	ng	179750	1	8.320	212752	20.0
Benzophenone	16.269	14.6	ng	408527	3	14.930	559738	20.0
n-Hexadecanoic ...	18.514	3.9	ng	151869	4	17.668	781020	20.0
4H-Cyclopenta[d...]	18.731	3.9	ng	153806	4	17.668	781020	20.0
11H-Benzo[b]flu...	20.541	3.3	ng	229428	5	21.962	1404880	20.0
11H-Benzo[a]flu...	20.640	2.1	ng	145079	5	21.962	1404880	20.0
n-Nonadecanol-1	21.545	5.1	ng	356859	5	21.962	1404880	20.0
Benzo[e]pyrene	24.577	2.3	ng	104581	6	25.406	913285	20.0
Perylene	25.082	6.7	ng	305739	6	25.406	913285	20.0