

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
 Data File : BP004827.D
 Acq On : 19 Feb 2021 17:56
 Operator : CG/JU
 Sample : M1440-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SP-227-233-B

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_P\Methods\8270E-BP020521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004827.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	286	290	297	rBV	25383	35692	1.32%	0.214%
2	5.358	362	369	381	rBV	987339	1378982	51.01%	8.284%
3	6.946	630	639	652	rBV	884967	1435854	53.11%	8.625%
4	7.757	769	777	786	rBV	193349	303497	11.23%	1.823%
5	8.916	966	974	984	rBV	531350	883184	32.67%	5.305%
6	10.551	1244	1252	1259	rBV	233479	388252	14.36%	2.332%
7	12.304	1527	1550	1568	rBV3	53074	285337	10.55%	1.714%
8	13.028	1666	1673	1680	rBV	1274783	1867599	69.08%	11.219%
9	13.863	1809	1815	1825	rBV	47958	72672	2.69%	0.437%
10	14.404	1901	1907	1914	rBV	320762	491389	18.18%	2.952%
11	15.904	2154	2162	2169	rBV	992885	1390019	51.41%	8.350%
12	17.163	2370	2376	2380	rBV	395626	578342	21.39%	3.474%
13	17.204	2380	2383	2389	rVB	177199	231193	8.55%	1.389%
14	17.292	2394	2398	2404	rVB	35451	53520	1.98%	0.322%
15	17.569	2437	2445	2450	rBV2	15149	28414	1.05%	0.171%
16	18.033	2519	2524	2525	rBV	27261	29234	1.08%	0.176%
17	18.057	2525	2528	2530	rVV2	29857	33131	1.23%	0.199%
18	18.222	2550	2556	2560	rBV2	32854	60099	2.22%	0.361%
19	18.516	2602	2606	2610	rBV	18745	29767	1.10%	0.179%
20	18.922	2671	2675	2680	rBV3	18182	30887	1.14%	0.186%
21	19.057	2694	2698	2706	rBV	20055	30522	1.13%	0.183%
22	19.175	2713	2718	2724	rBV	349366	459240	16.99%	2.759%
23	19.498	2769	2773	2774	rBV	53843	59912	2.22%	0.360%
24	19.527	2774	2778	2786	rVV	298158	419837	15.53%	2.522%
25	19.727	2805	2812	2817	rBV	2256895	2703541	100.00%	16.241%
26	20.169	2883	2887	2890	rVB3	20748	28576	1.06%	0.172%
27	20.692	2972	2976	2980	rBV	109371	129235	4.78%	0.776%
28	20.739	2981	2984	2989	rVB	40939	56322	2.08%	0.338%
29	20.957	3016	3021	3030	rBV6	118268	215081	7.96%	1.292%
30	21.027	3030	3033	3041	rVB	40051	63630	2.35%	0.382%
31	21.245	3064	3070	3074	rBV2	633404	1025253	37.92%	6.159%
32	21.286	3074	3077	3083	rVB	162933	205591	7.60%	1.235%
33	21.386	3090	3094	3102	rVB8	64015	122710	4.54%	0.737%
34	22.710	3315	3319	3325	rVB3	101819	156876	5.80%	0.942%
35	22.851	3339	3343	3349	rBV	116773	275696	10.20%	1.656%
36	23.351	3425	3428	3436	rVB	77413	134979	4.99%	0.811%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.445	3440	3444	3454	rVB	116328	241684	8.94%	1.452%
38	23.551	3456	3462	3469	rBV2	365499	711125	26.30%	4.272%

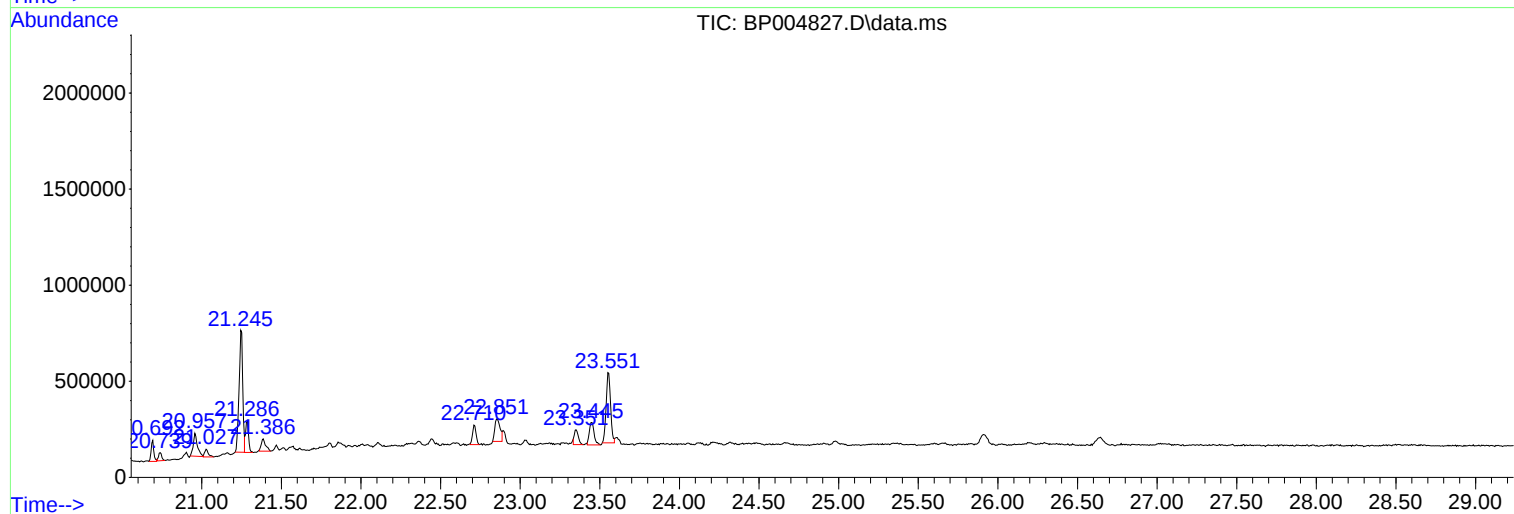
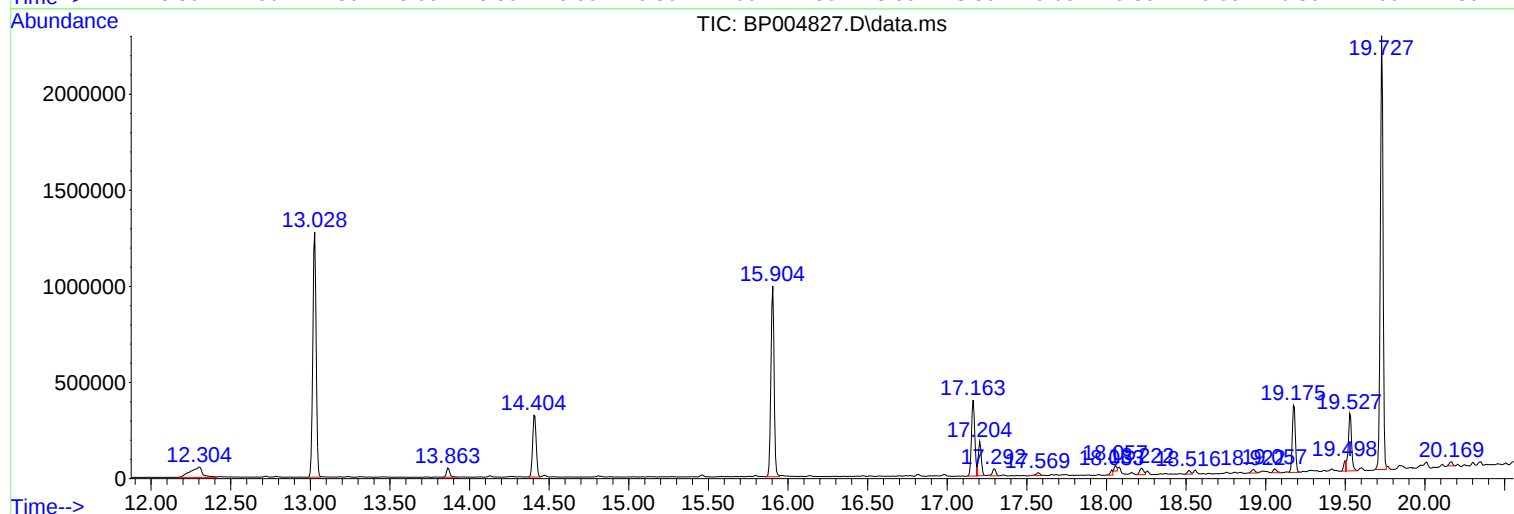
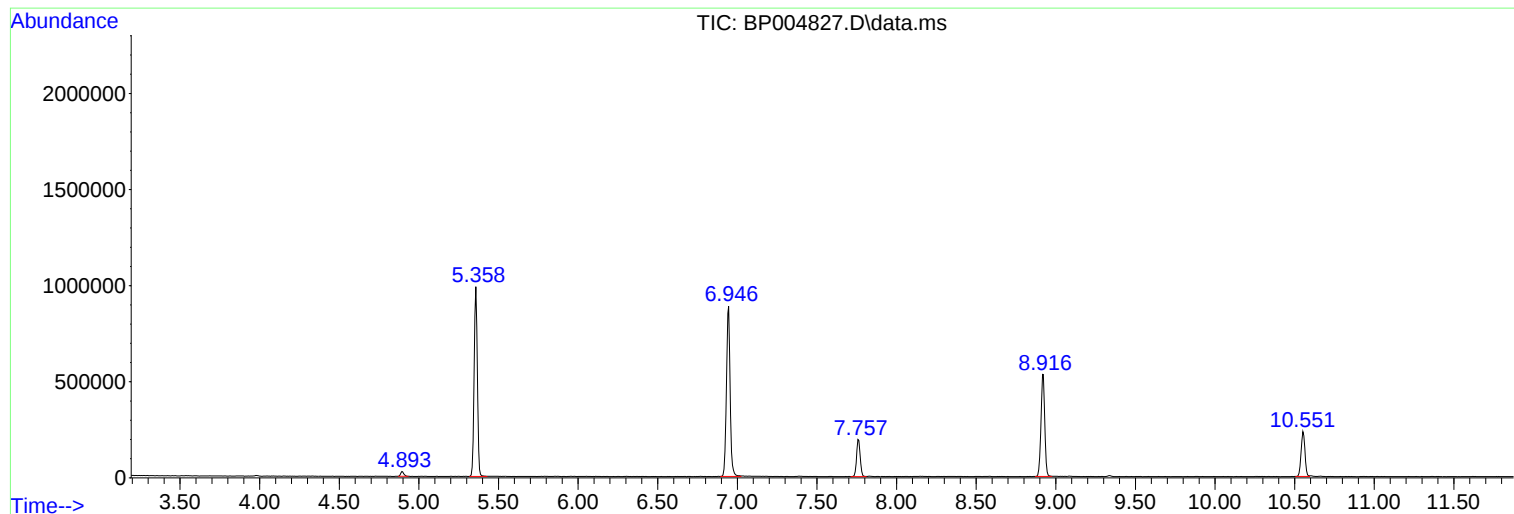
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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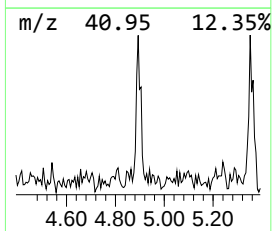
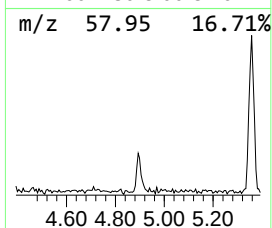
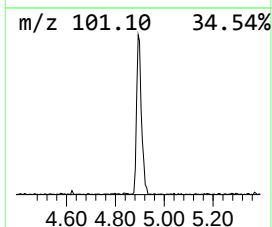
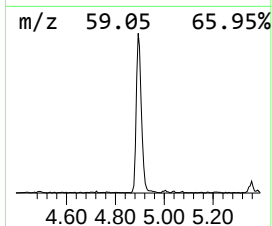
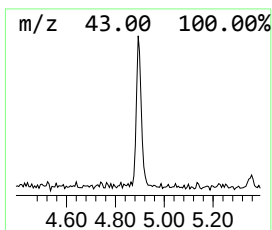
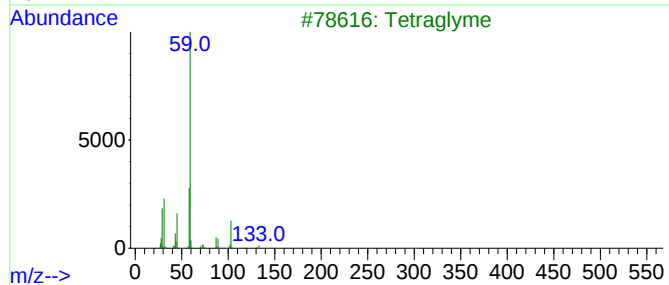
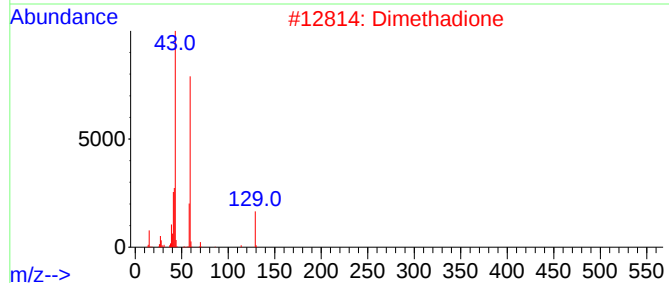
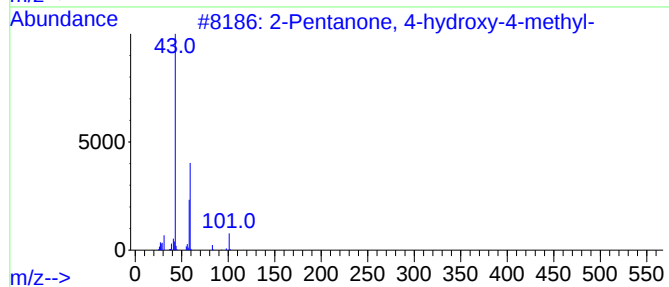
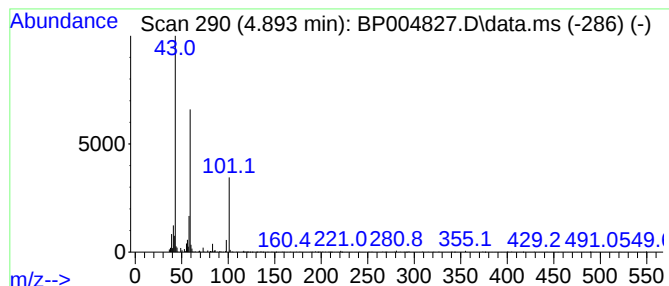
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	2.35 ng	35692	1,4-Dichlorobenzene-d4	7.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39	
2	Dimethadione	129	C5H7NO3	000695-53-4	33	
3	Tetraglyme	222	C10H22O5	000143-24-8	32	
4	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28	
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	



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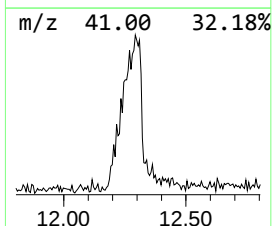
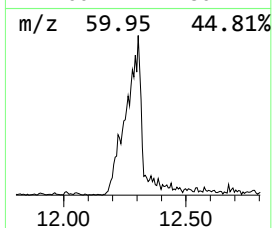
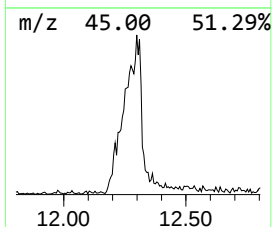
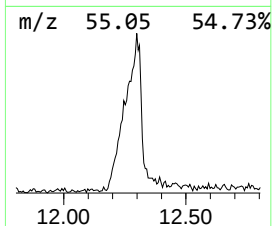
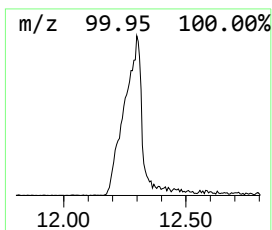
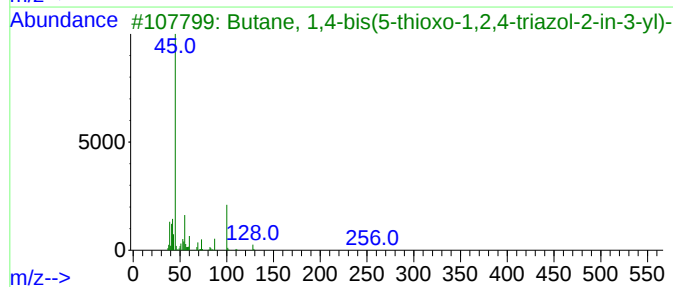
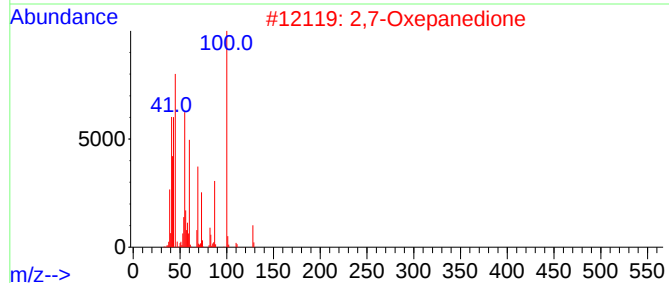
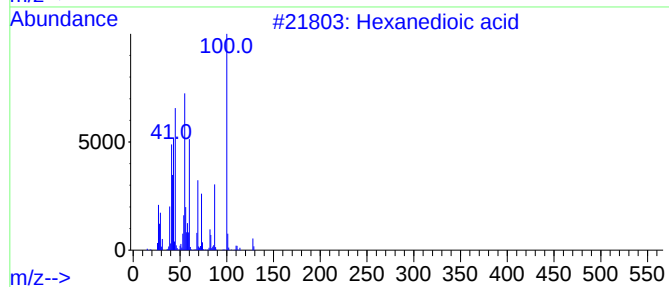
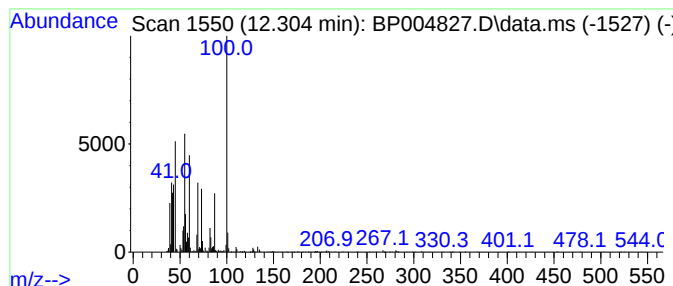
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Hexanedioic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	14.70 ng	285337	Naphthalene-d8	10.552

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid	146	C6H10O4	000124-04-9	90
2			2,7-Oxepanedione	128	C6H8O3	002035-75-8	72
3			Butane, 1,4-bis(5-thioxo-1,2,4-t...	256	C8H12N6S2	007271-37-6	64
4			Proline, 3-hydroxy-4-methyl-	145	C6H11NO3	077647-24-6	38
5			N-[[2-Morpholino]ethyl]succinami...	230	C10H18N2O4	342021-41-4	35



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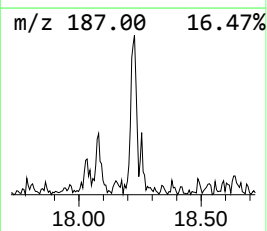
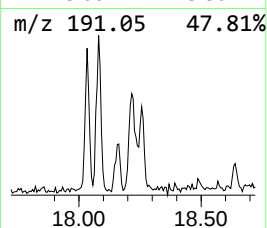
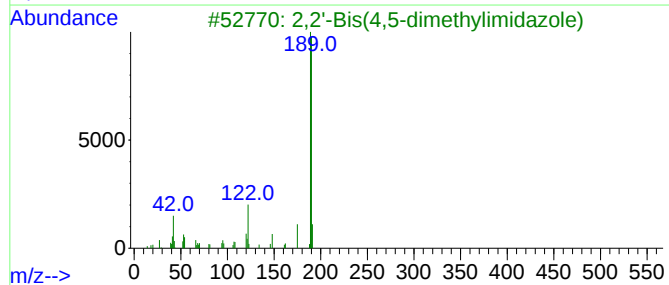
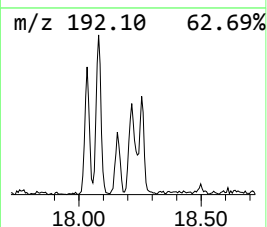
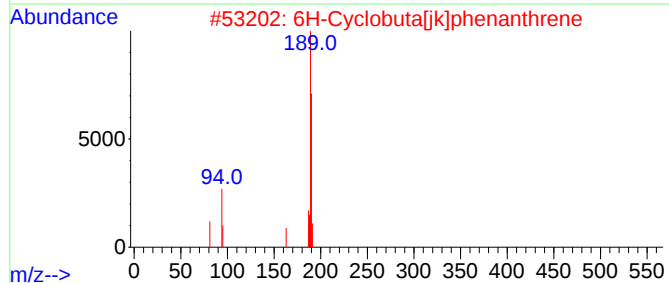
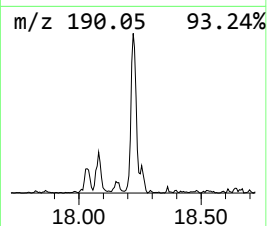
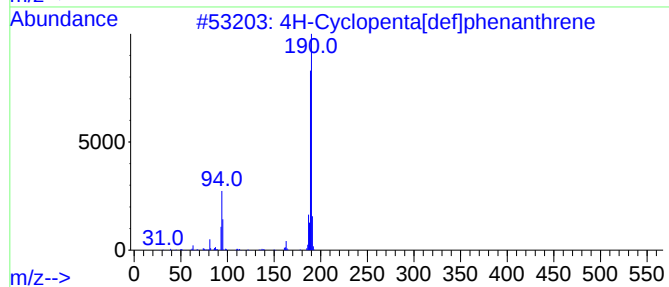
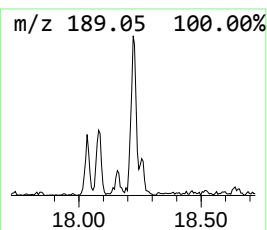
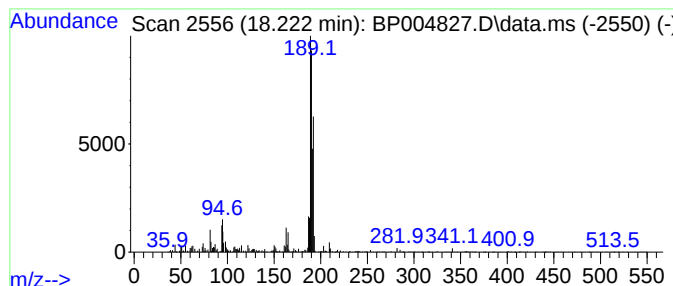
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	2.08 ng	60099	Phenanthrene-d10	17.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	47
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	43
4			3,5-Dichlorobenzoic acid	190	C7H4Cl2O2	000051-36-5	30
5			1,3-Dioxolo[4,5-g]isoquinoline, ...	341	C20H23NO4	005544-49-0	30



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ClientSampleId :
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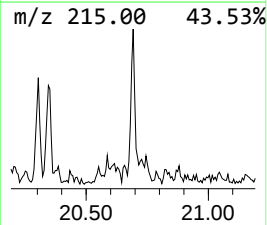
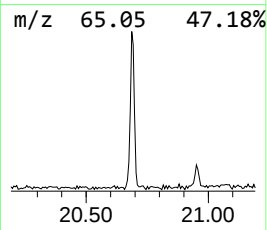
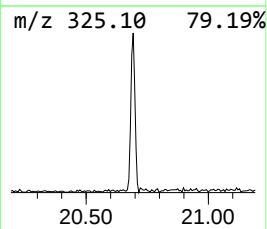
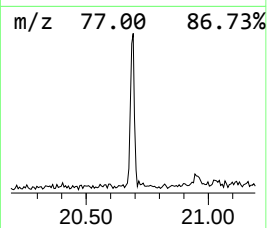
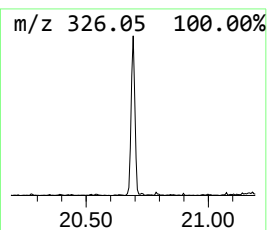
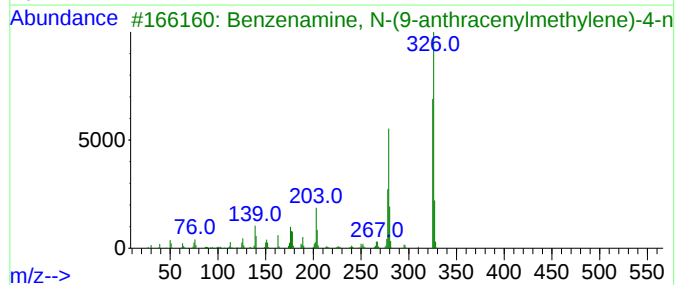
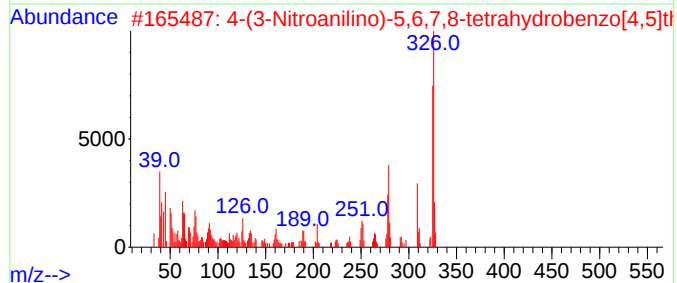
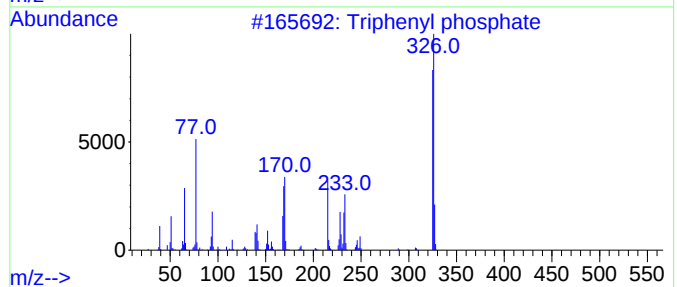
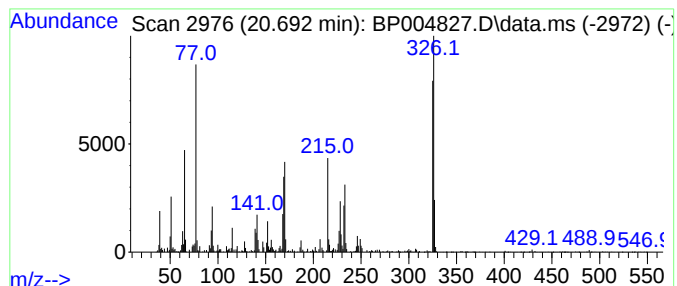
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Triphenyl phosphate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.692	2.52 ng	129235	Chrysene-d12	21.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenyl phosphate	326	C18H15O4P	000115-86-6	99
2			4-(3-Nitroanilino)-5,6,7,8-tetra...	326	C16H14N4O2S	313952-58-8	14
3			Benzenamine, N-(9-anthracenylmet...	326	C21H14N2O2	014607-12-6	11
4			Furo[2,3-H]coumarine, 1-(4-chlor...	325	C18H12ClNO3	1000270-16-3	9
5			1,2-Benzisothiazol-3(2H)-one, 4,...	325	C13H7N7O2S	1000276-62-9	9



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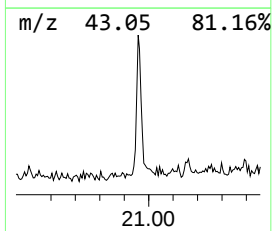
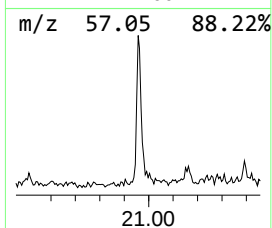
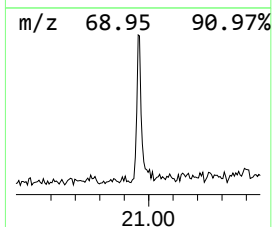
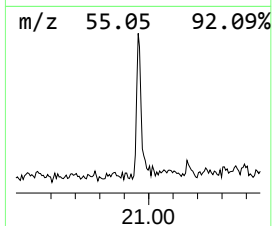
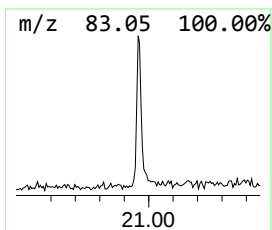
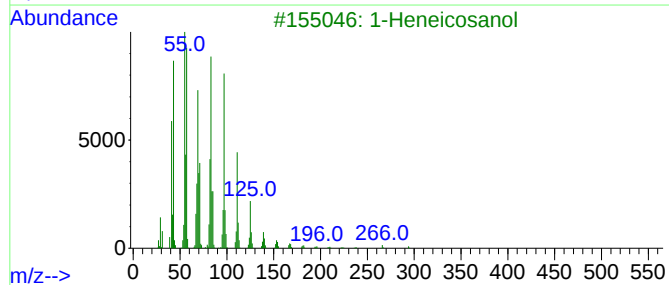
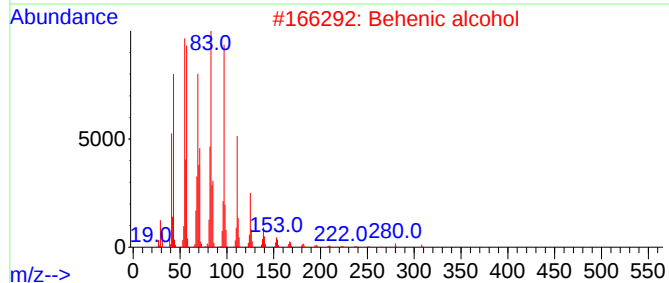
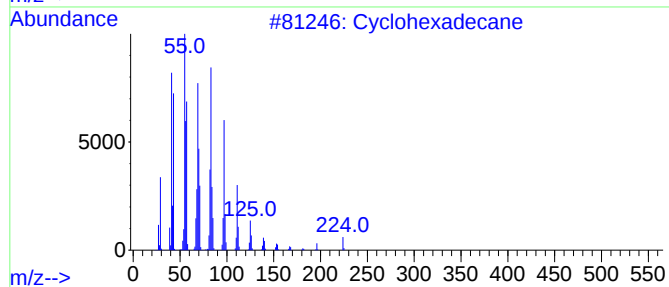
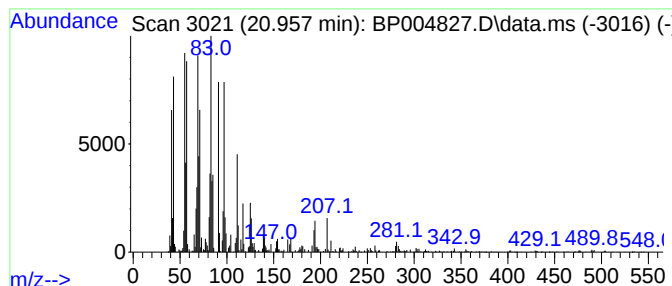
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	4.20 ng	215081	Chrysene-d12	21.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	96
2			Behenic alcohol	326	C22H46O	000661-19-8	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			17-Pentatriacontene	491	C35H70	006971-40-0	93
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
Data File : BP004827.D
Acq On : 19 Feb 2021 17:56
Operator : CG/JU
Sample : M1440-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-227-233-B

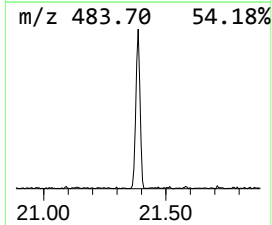
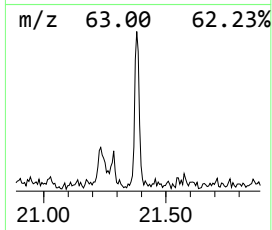
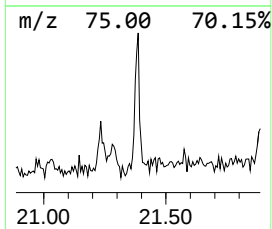
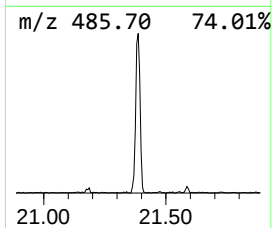
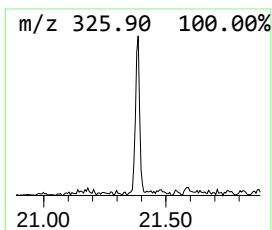
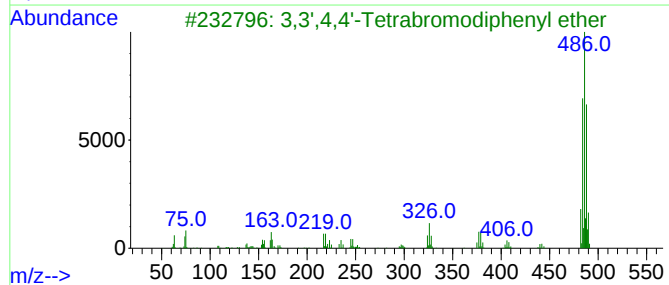
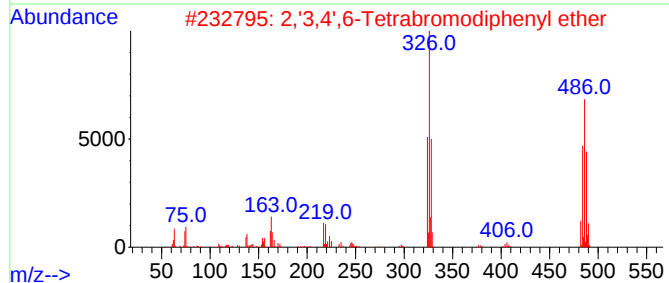
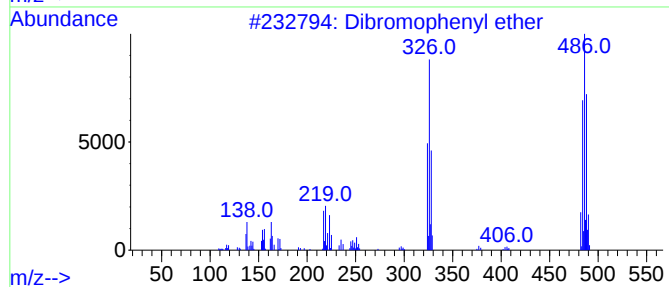
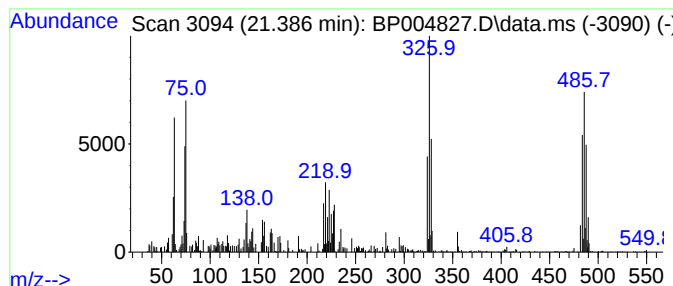
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Dibromophenyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.386	2.39 ng	122710	Chrysene-d12	21.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibromophenyl ether	482	C12H6Br4O	005436-43-1	94
2			2,'3,4',6-Tetrabromodiphenyl ether	482	C12H6Br4O	189084-62-6	89
3			3,3',4,4'-Tetrabromodiphenyl ether	482	C12H6Br4O	093703-48-1	47
4			2,3',4,4',5'-Pentachloro-1,1'-bi...	324	C12H5Cl5	065510-44-3	25
5			2,3,3',4',5'- Pentachloro-1,1'-b...	324	C12H5Cl5	076842-07-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
Data File : BP004827.D
Acq On : 19 Feb 2021 17:56
Operator : CG/JU
Sample : M1440-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-227-233-B

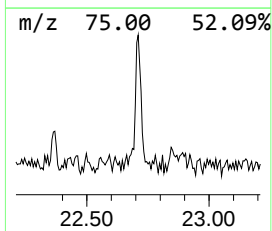
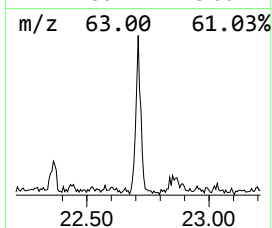
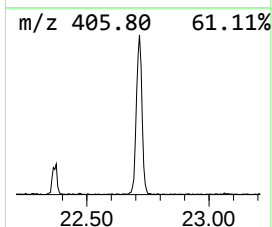
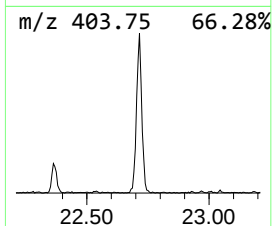
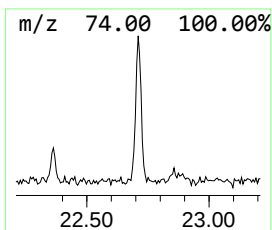
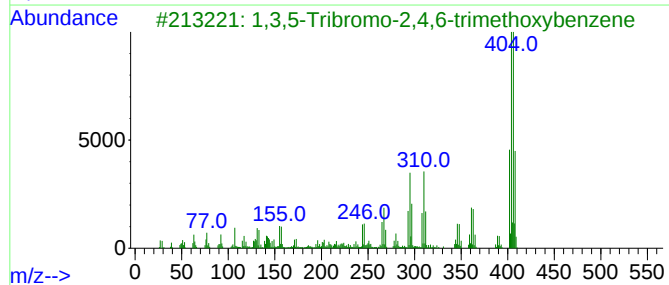
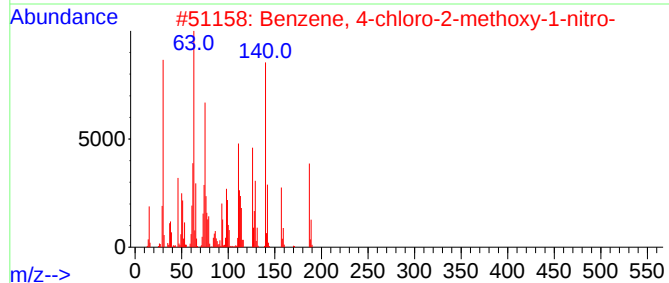
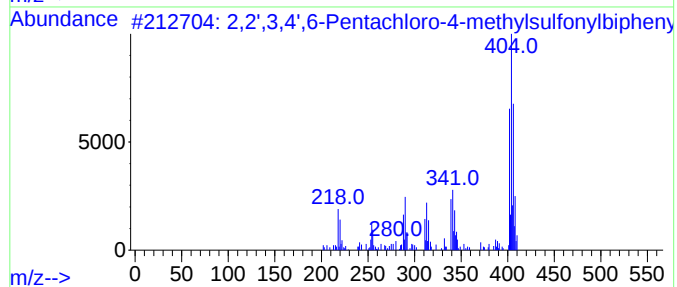
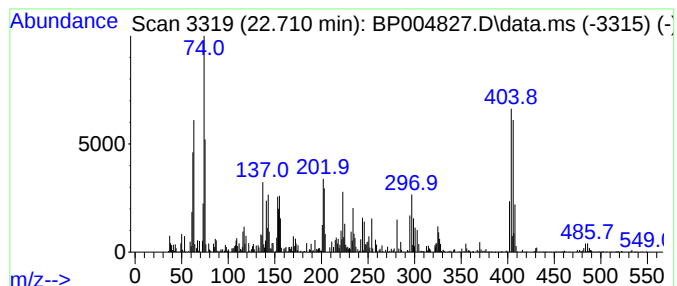
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown22.710 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.710	4.41 ng	156876	Perylene-d12	23.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2',3,4',6-Pentachloro-4-methyl...	402	C13H7Cl5O2S	149949-87-1	47		
2	Benzene, 4-chloro-2-methoxy-1-ni...	187	C7H6ClNO3	006627-53-8	27		
3	1,3,5-Tribromo-2,4,6-trimethoxyb...	402	C9H9Br3O3	105404-90-8	25		
4	2-Chloroethyl carbonate	186	C5H8Cl2O3	000623-97-2	25		
5	Thiocyanic acid, 2,4-dinitrophen...	225	C7H3N3O4S	001594-56-5	23		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
Data File : BP004827.D
Acq On : 19 Feb 2021 17:56
Operator : CG/JU
Sample : M1440-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-227-233-B

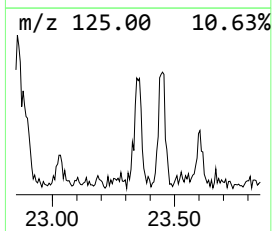
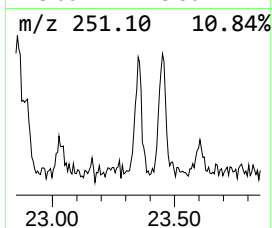
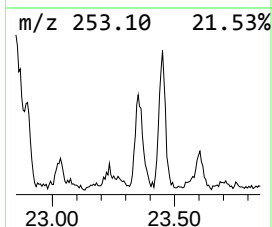
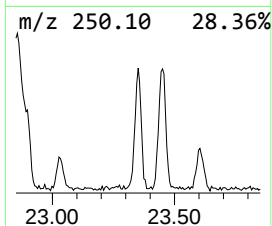
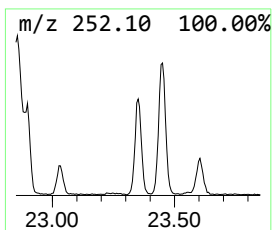
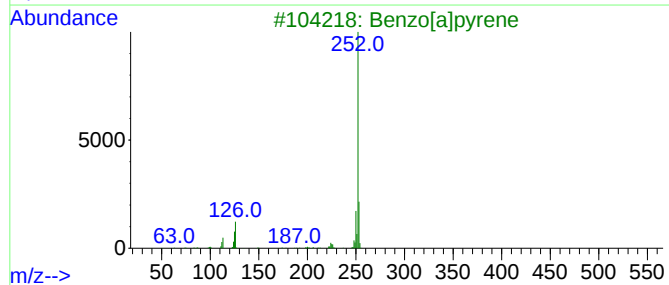
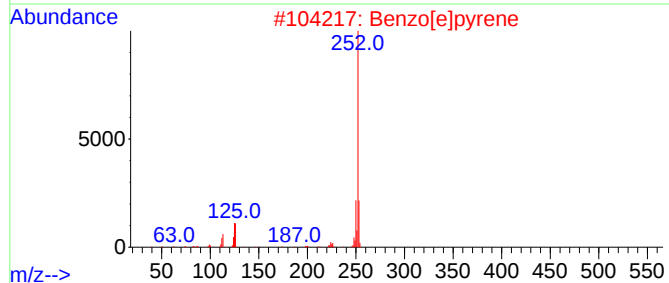
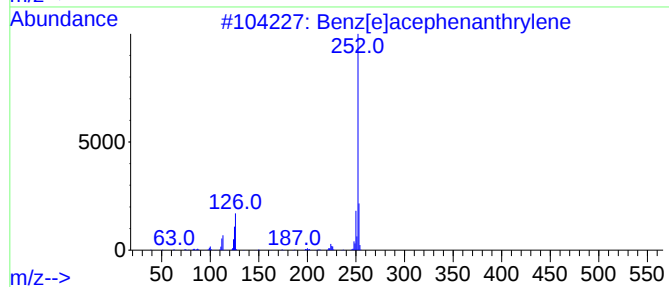
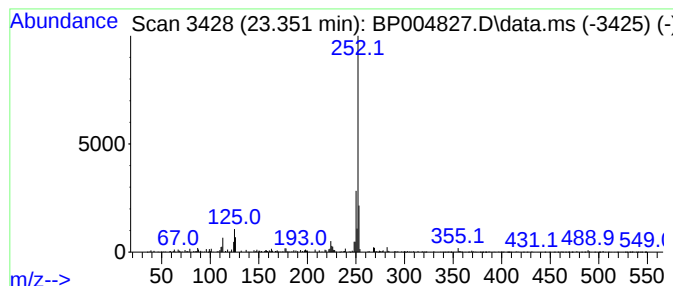
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.351	3.80 ng	134979	Perylene-d12	23.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	91
2			Benzo[e]pyrene	252	C20H12	000192-97-2	90
3			Benzo[a]pyrene	252	C20H12	000050-32-8	90
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	81
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021921\
Data File : BP004827.D
Acq On : 19 Feb 2021 17:56
Operator : CG/JU
Sample : M1440-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-227-233-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.893	2.4	ng	35692	1	7.763	303497	20.0
Hexanedioic acid	12.304	14.7	ng	285337	2	10.552	388252	20.0
4H-Cyclopenta[d]...	18.222	2.1	ng	60099	4	17.163	578342	20.0
Triphenyl phosph...	20.692	2.5	ng	129235	5	21.251	1025250	20.0
Cyclohexadecane	20.957	4.2	ng	215081	5	21.251	1025250	20.0
Dibromophenyl e...	21.386	2.4	ng	122710	5	21.251	1025250	20.0
unknown22.710	22.710	4.4	ng	156876	6	23.551	711125	20.0
Benzo[e]pyrene	23.351	3.8	ng	134979	6	23.551	711125	20.0