

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092321\
 Data File : BP007142.D
 Acq On : 24 Sep 2021 01:01
 Operator : CG/JU
 Sample : M3797-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20430

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-BP092121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007142.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.469	398	405	417	rBV	4372596	6521279	52.71%	4.686%
2	7.063	667	676	692	rBV	4031040	6537137	52.84%	4.697%
3	7.893	809	817	825	rBV	1091102	1731563	14.00%	1.244%
4	9.052	1006	1014	1025	rBV	2453812	4073355	32.93%	2.927%
5	10.475	1249	1256	1266	rBV	254682	480435	3.88%	0.345%
6	10.693	1282	1293	1299	rBV	1418432	2476867	20.02%	1.780%
7	12.351	1569	1575	1582	rVB	119568	216722	1.75%	0.156%
8	12.569	1606	1612	1616	rBV	134435	231212	1.87%	0.166%
9	13.145	1702	1710	1720	rBV	6117944	8985675	72.63%	6.457%
10	13.310	1731	1738	1740	rBV6	77331	162112	1.31%	0.116%
11	13.792	1817	1820	1824	rBV5	95820	156276	1.26%	0.112%
12	13.845	1825	1829	1830	rVV	174705	241395	1.95%	0.173%
13	13.869	1830	1833	1842	rVB	594528	994719	8.04%	0.715%
14	14.010	1854	1857	1860	rVB	166319	194293	1.57%	0.140%
15	14.245	1894	1897	1902	rBV	198925	352009	2.85%	0.253%
16	14.351	1912	1915	1922	rVB5	326248	580231	4.69%	0.417%
17	14.522	1935	1944	1950	rBV	2215742	3939178	31.84%	2.831%
18	14.587	1951	1955	1963	rVB	483189	851752	6.88%	0.612%
19	15.045	2030	2033	2037	rVB4	191402	237982	1.92%	0.171%
20	15.310	2075	2078	2082	rVB2	338103	404962	3.27%	0.291%
21	15.569	2118	2122	2133	rVB	759576	1519704	12.28%	1.092%
22	16.010	2192	2197	2204	rBV	4880302	6849678	55.37%	4.922%
23	16.263	2236	2240	2245	rVB	1207069	1782151	14.41%	1.281%
24	17.086	2376	2380	2389	rVB	2141421	3313046	26.78%	2.381%
25	17.269	2407	2411	2415	rBV	2389488	3781844	30.57%	2.718%
26	17.316	2415	2419	2426	rVV	5573865	8162175	65.98%	5.865%
27	17.404	2430	2434	2439	rVB	1337419	1908736	15.43%	1.372%
28	19.280	2748	2753	2760	rVB	9056973	12371376	100.00%	8.890%
29	19.633	2804	2813	2820	rVB	7674709	12262813	99.12%	8.812%
30	19.827	2842	2846	2850	rVB	8295498	10257884	82.92%	7.371%
31	20.110	2891	2894	2899	rVB	1464692	1991544	16.10%	1.431%
32	20.210	2908	2911	2915	rVB	1163903	1374942	11.11%	0.988%
33	21.345	3099	3104	3109	rBV3	4913315	10049571	81.23%	7.221%
34	21.392	3109	3112	3121	rVB	3963251	5130638	41.47%	3.687%
35	21.510	3129	3132	3139	rVB	837909	1132456	9.15%	0.814%
36	23.027	3385	3390	3395	rBV	2610709	5907316	47.75%	4.245%

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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-BP092121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.551	3474	3479	3489	rVB	1748144	3627323	29.32%	2.607%
38	23.657	3491	3497	3504	rVB	2629322	5098561	41.21%	3.664%
39	23.763	3510	3515	3521	rBV2	1736553	3272419	26.45%	2.351%

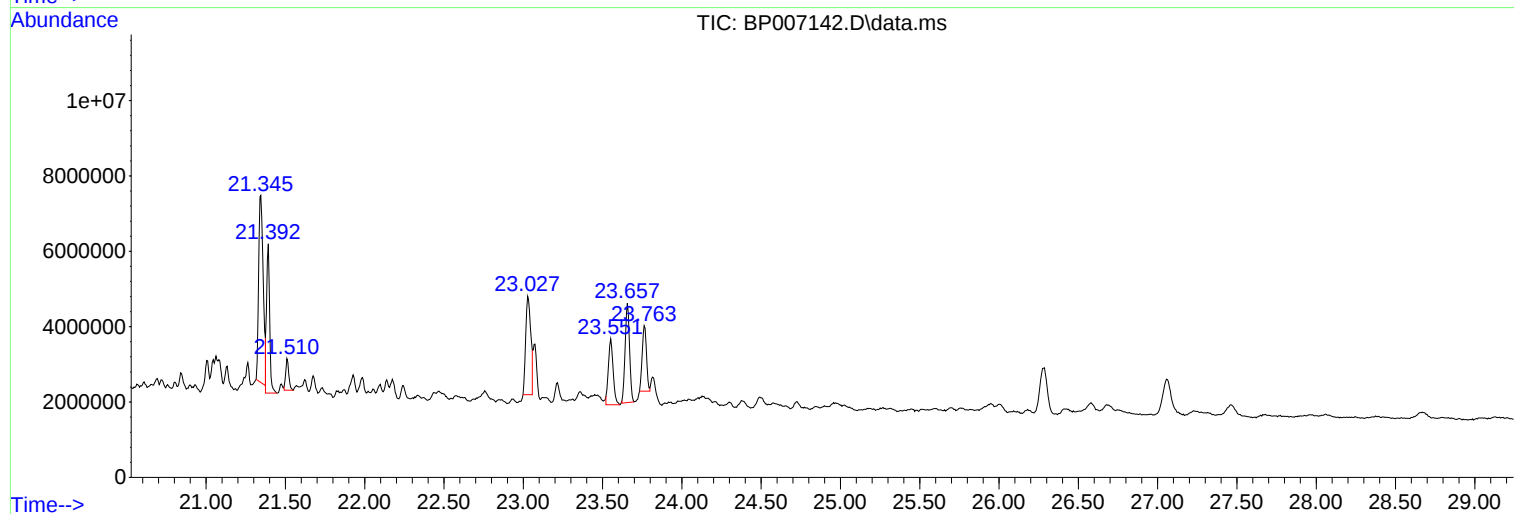
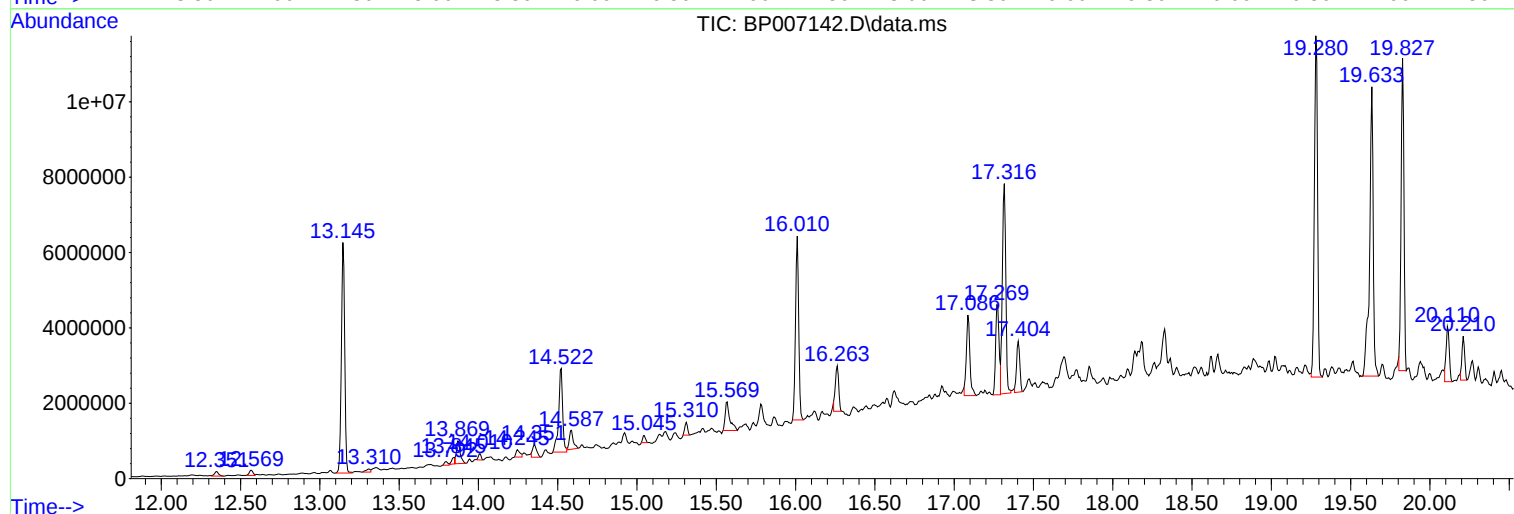
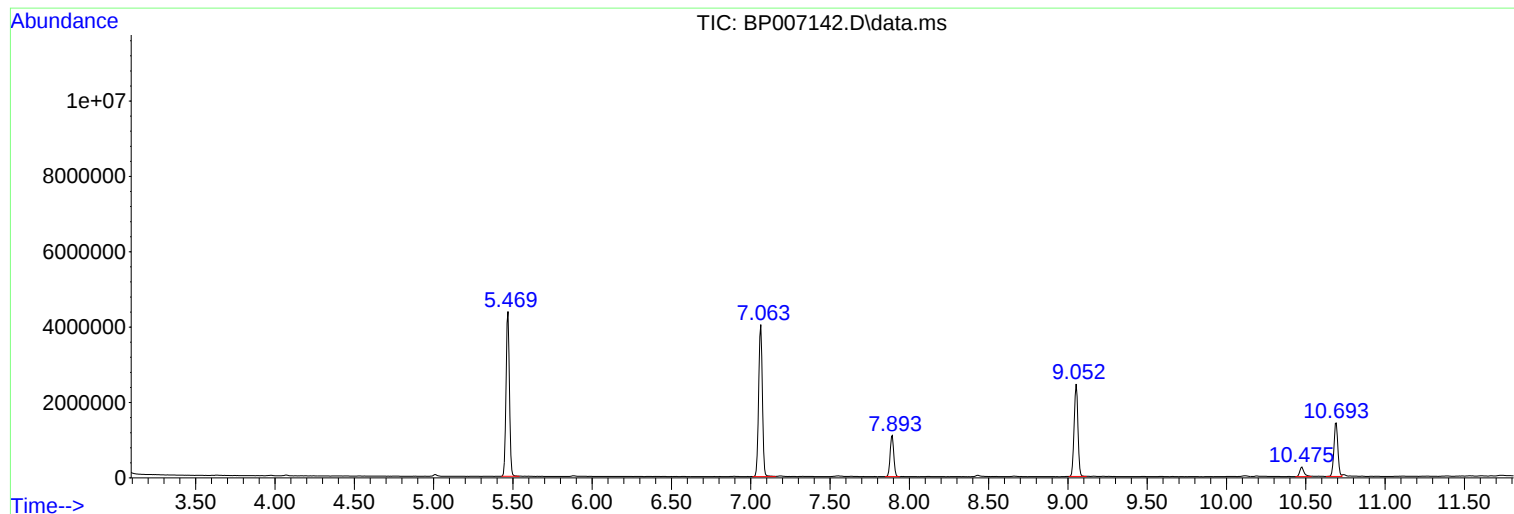
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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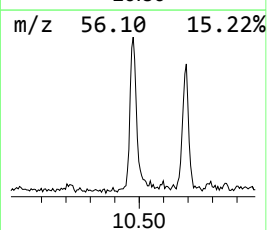
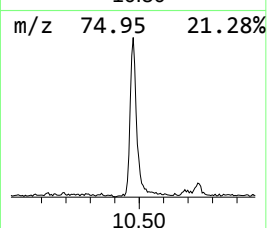
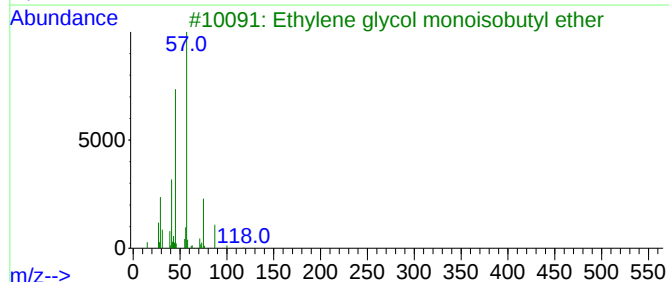
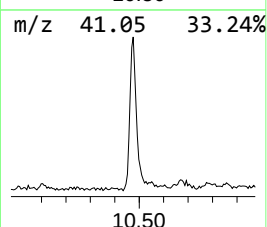
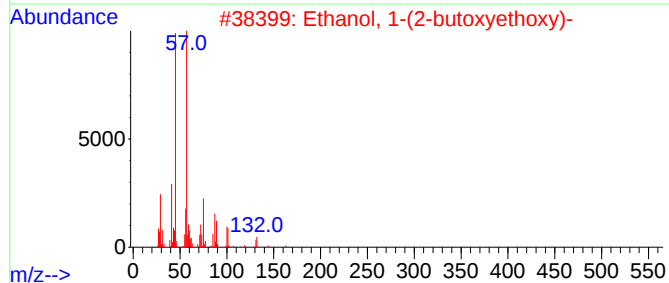
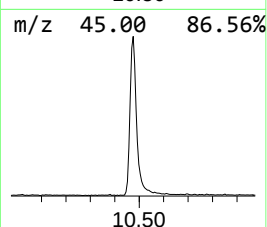
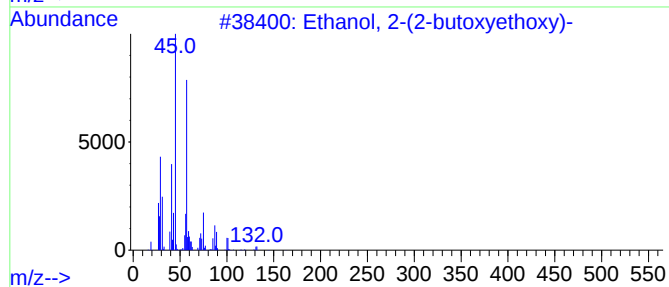
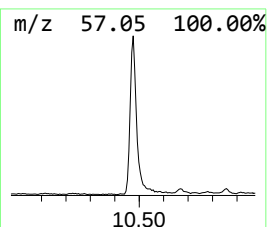
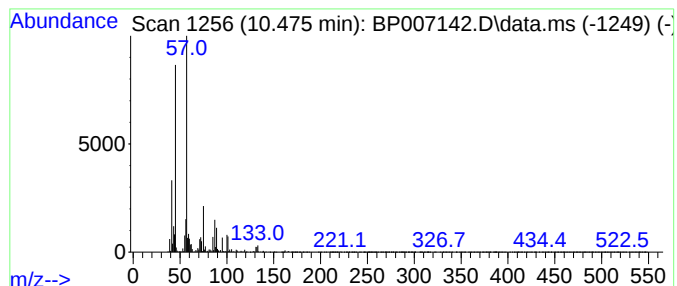
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.88 ng	480435	Naphthalene-d8	10.693

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



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ALS Vial : 15 Sample Multiplier: 1

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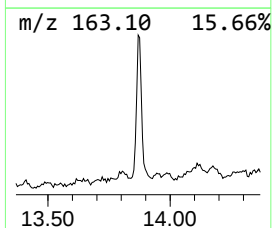
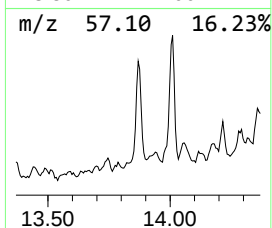
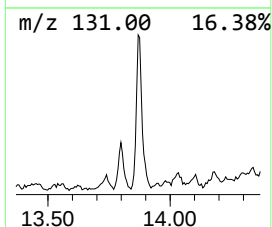
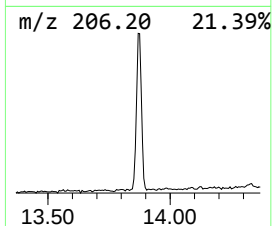
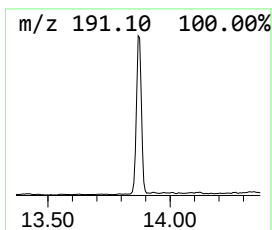
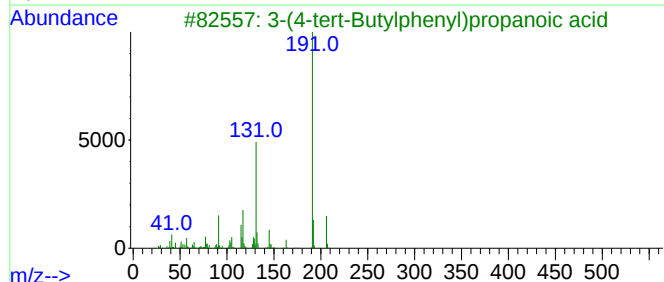
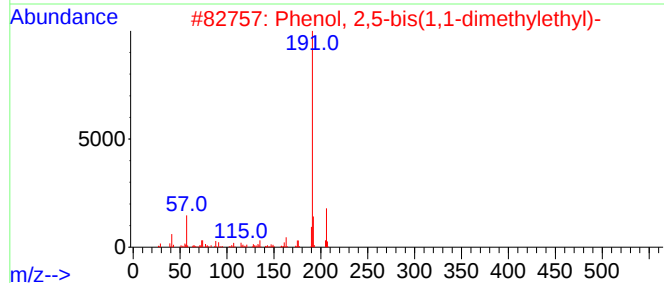
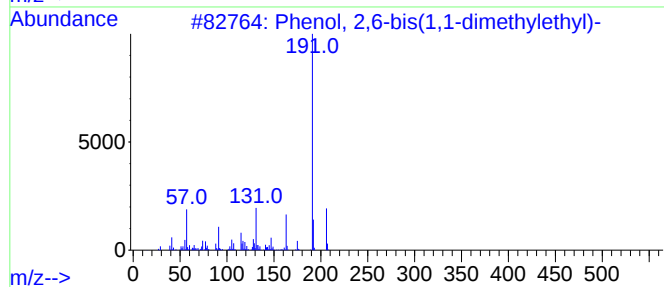
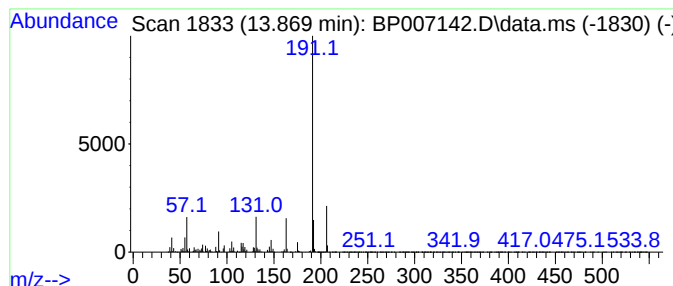
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.869	5.05 ng	994719	Acenaphthene-d10	14.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	94
2			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	81
3			3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	81
4			1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	80
5			Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	74



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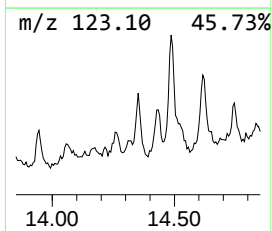
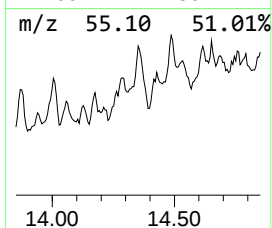
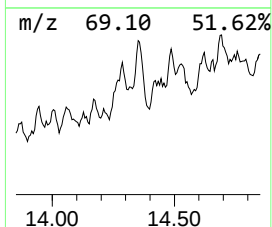
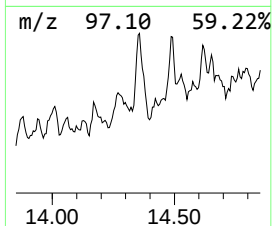
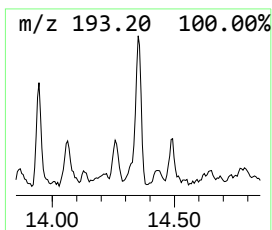
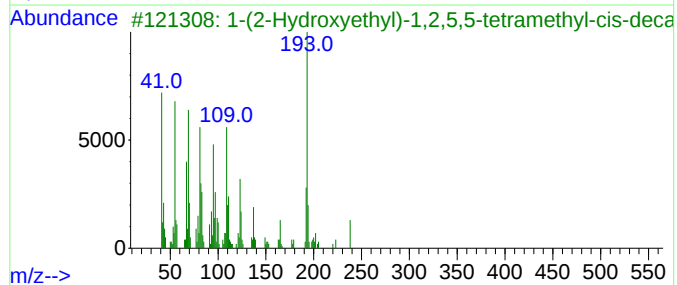
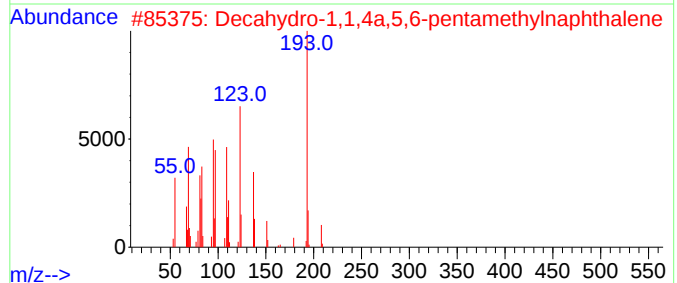
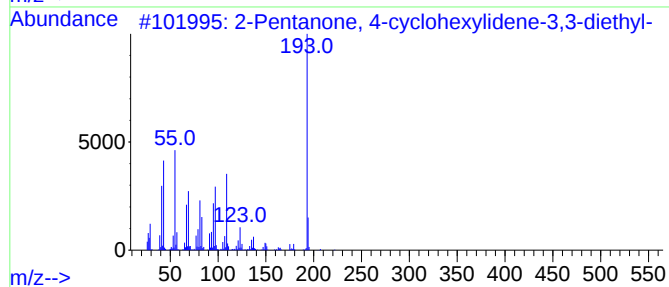
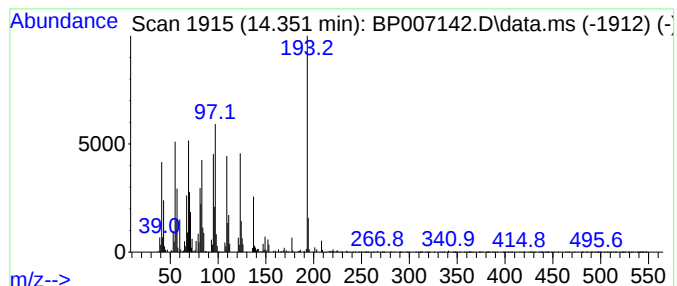
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown14.351 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.351	2.95 ng	580231	Acenaphthene-d10	14.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	49
2			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	46
3			1-(2-Hydroxyethyl)-1,2,5,5-tetra...	238	C16H30O	1010298-97-4	43
4			Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	37
5			Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	25



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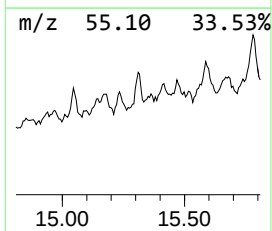
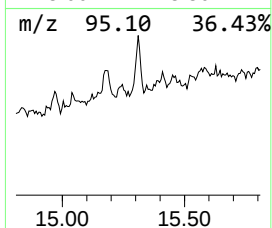
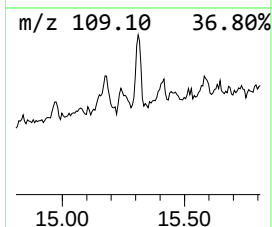
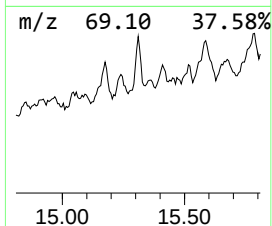
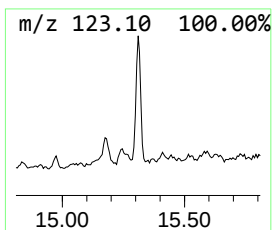
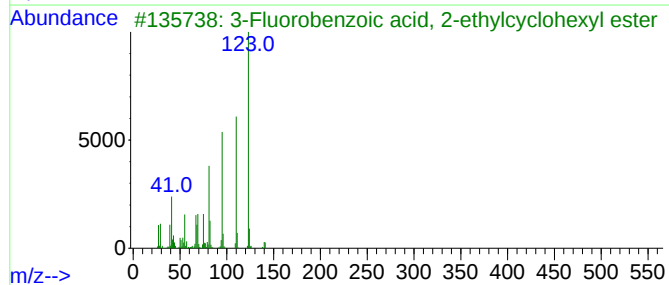
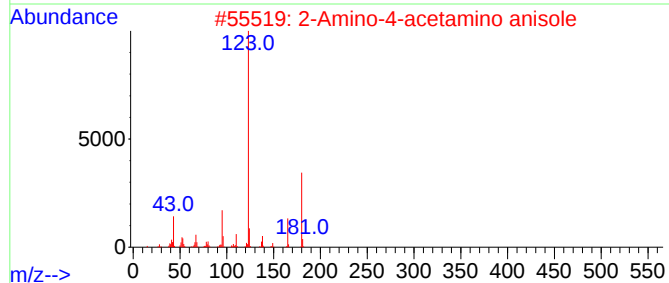
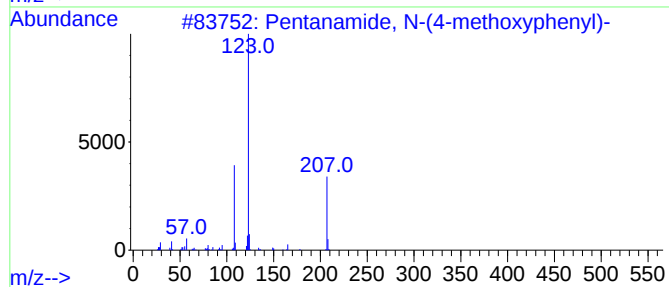
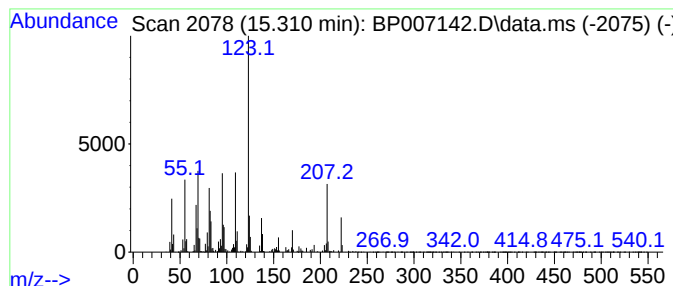
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown15.310 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.310	2.06 ng	404962	Acenaphthene-d10	14.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	49
2			2-Amino-4-acetamino anisole	180	C9H12N2O2	006375-47-9	47
3			3-Fluorobenzoic acid, 2-ethylcyclohexyl ester	250	C15H19FO2	1000279-04-9	47
4			4,4-Dimethoxy-2,5-cyclohexadiene-1-carboxylic acid	154	C8H10O3	000935-50-2	47
5			Ethanone, 1-[3-[2-methyl-2-(5-methyl-2-oxo-2,5-dihydrofuran-3-yl)propyl]phenyl]-	222	C13H18O3	080114-28-9	46



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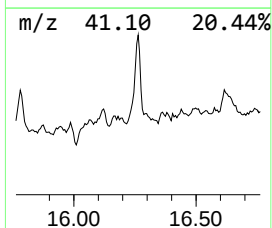
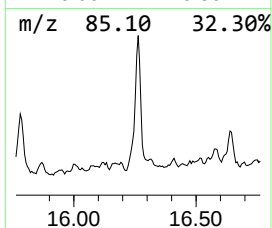
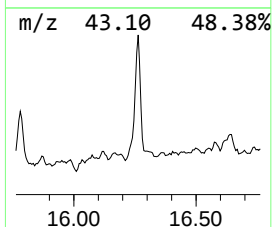
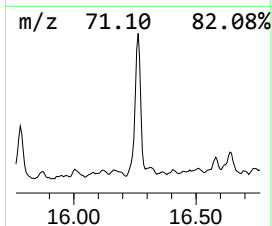
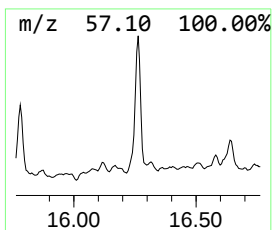
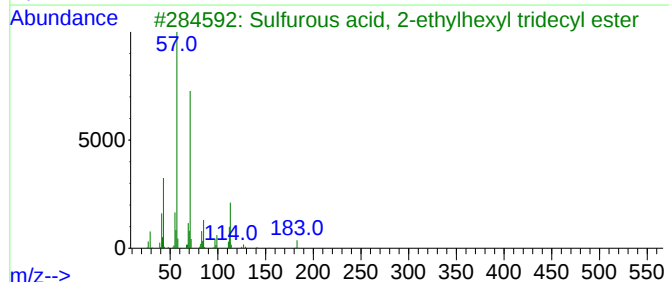
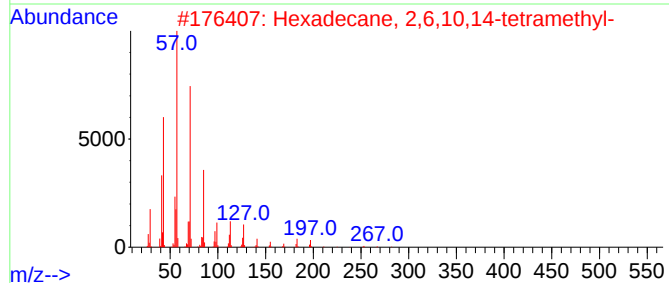
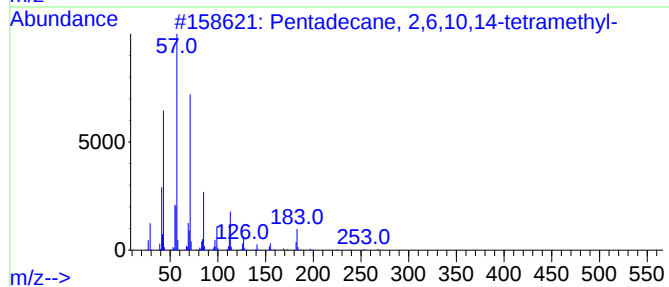
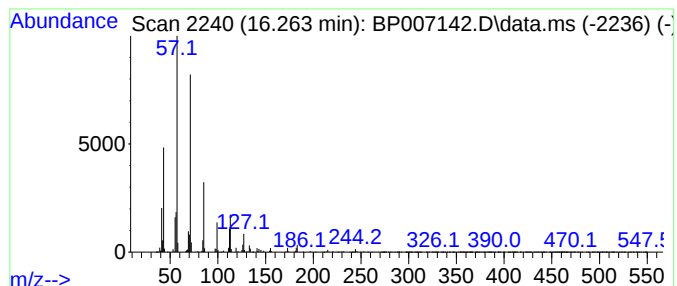
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecane, 2,6,10,14-tetr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.263	9.42 ng	1782150	Phenanthrene-d10	17.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	86
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
3			Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	80
4			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	74
5			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092321\
Data File : BP007142.D
Acq On : 24 Sep 2021 01:01
Operator : CG/JU
Sample : M3797-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

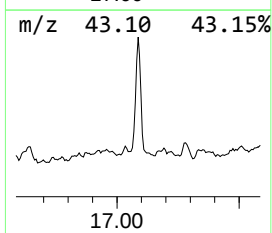
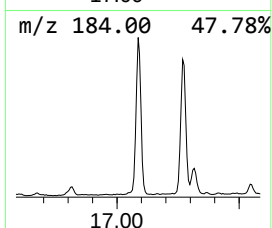
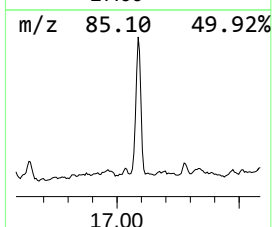
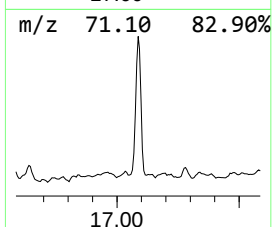
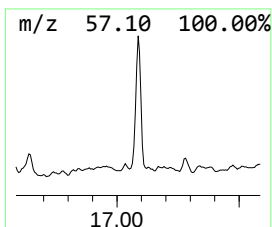
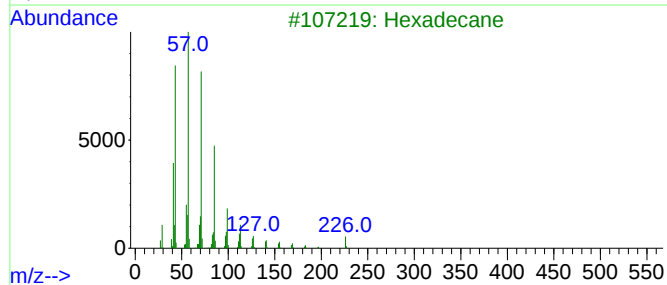
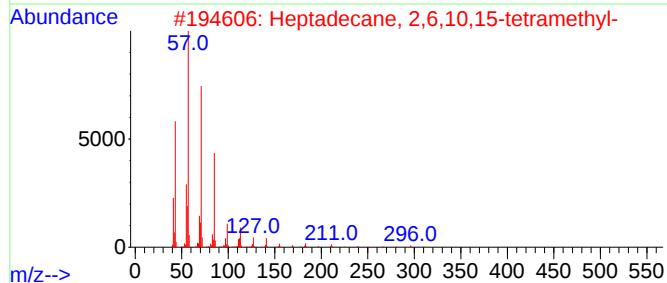
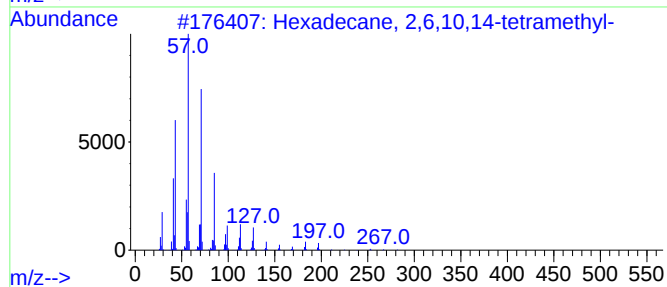
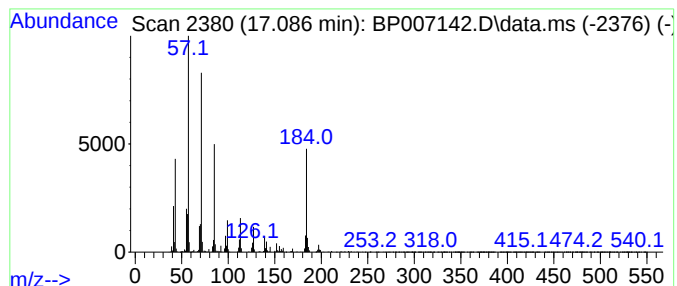
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane, 2,6,10,14-tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.086	17.52 ng	3313050	Phenanthrene-d10	17.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	81
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	68
3	Hexadecane	226	C16H34	000544-76-3	68
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	64
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092321\
Data File : BP007142.D
Acq On : 24 Sep 2021 01:01
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Sample : M3797-03
Misc :
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Instrument :
BNA_P
ClientSampleId :
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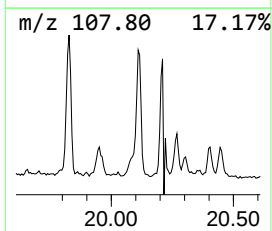
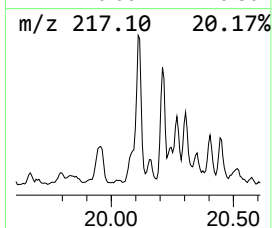
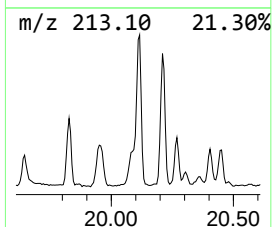
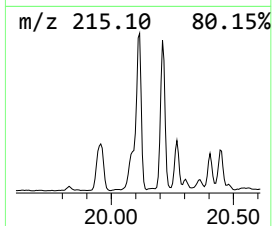
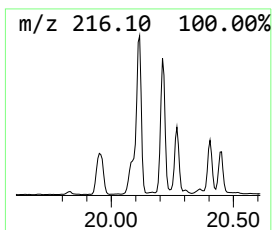
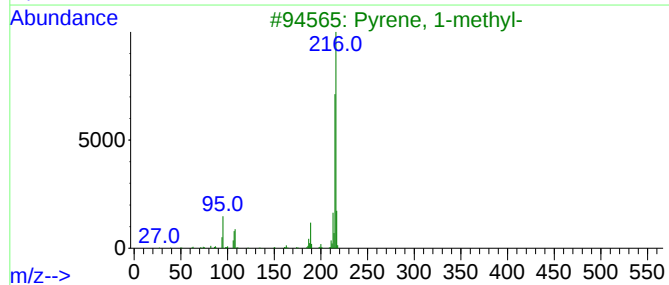
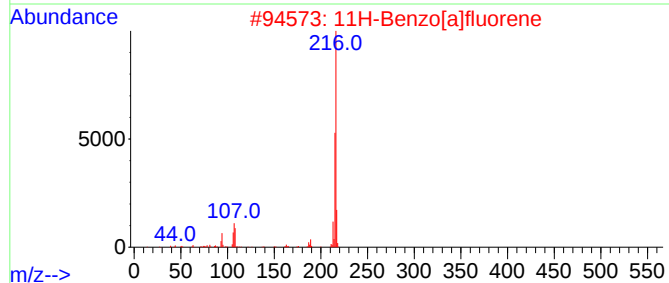
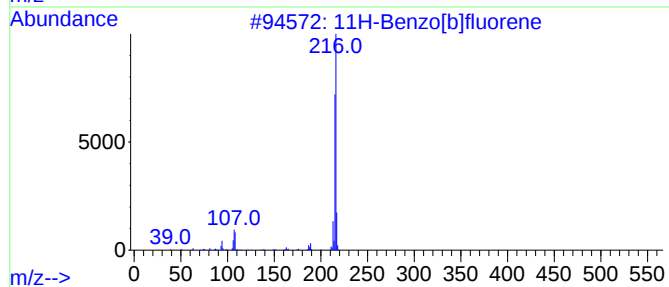
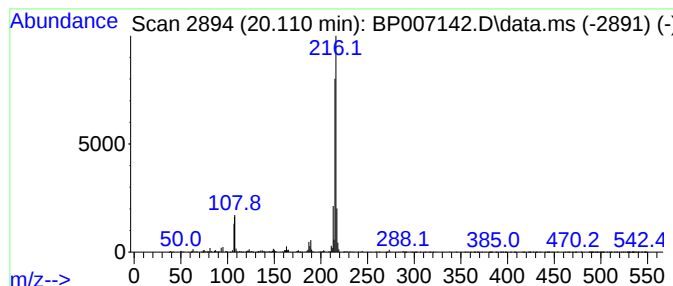
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.110	3.96 ng	1991540	Chrysene-d12	21.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
3			Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	76
5			Pyrene, 2-methyl-	216	C17H12	003442-78-2	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092321\
Data File : BP007142.D
Acq On : 24 Sep 2021 01:01
Operator : CG/JU
Sample : M3797-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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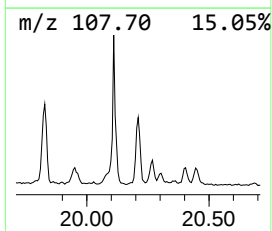
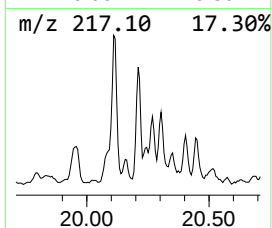
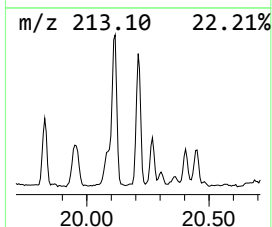
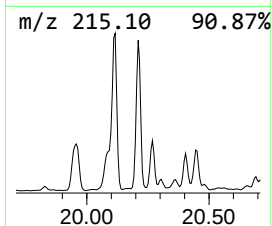
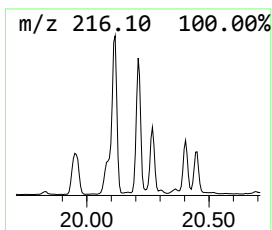
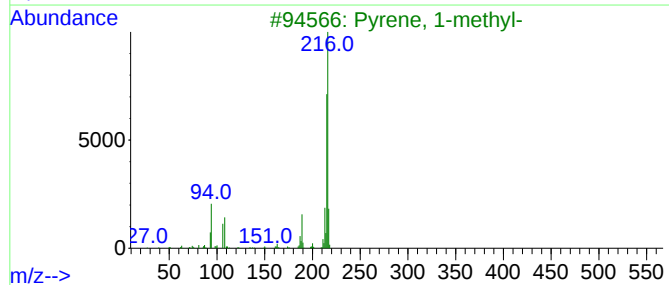
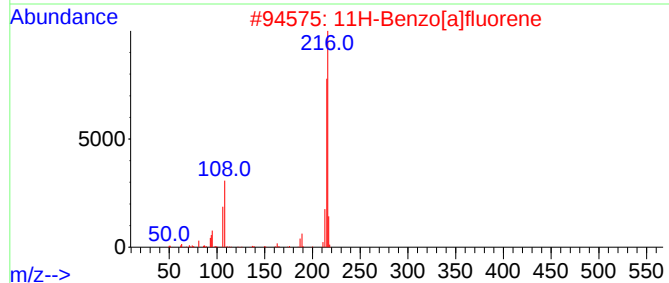
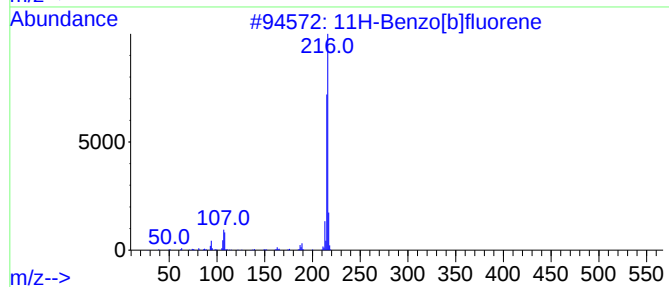
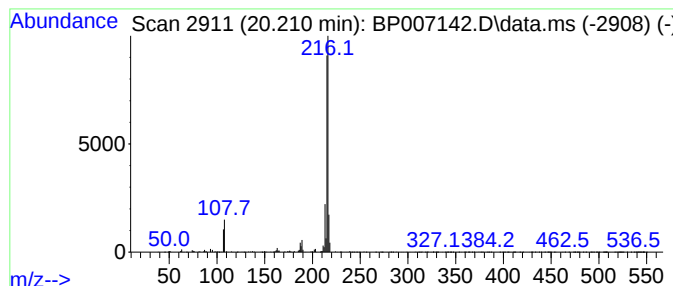
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.210	2.74 ng	1374940	Chrysene-d12	21.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
3			Pyrene, 1-methyl-	216	C17H12	002381-21-7	74
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	70
5			.beta.-Carboline, 1,2,3,4-tetra...	260	C14H16N2O3	029573-11-3	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092321\
Data File : BP007142.D
Acq On : 24 Sep 2021 01:01
Operator : CG/JU
Sample : M3797-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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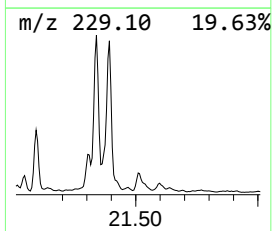
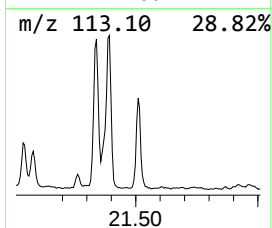
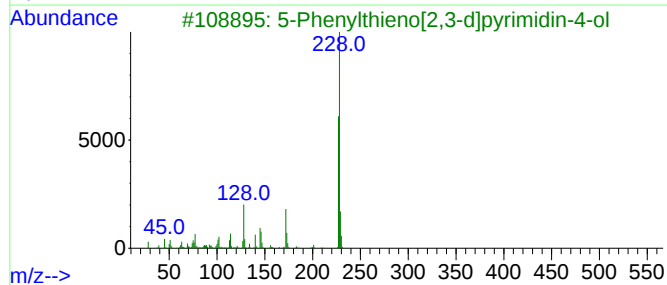
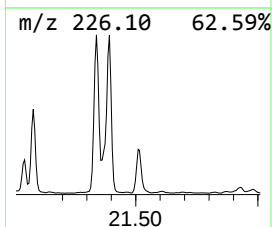
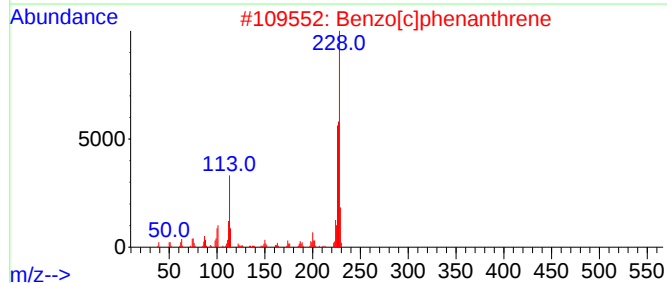
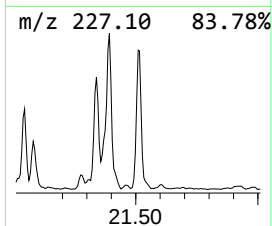
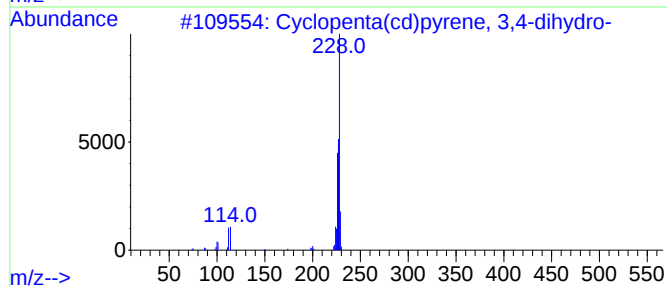
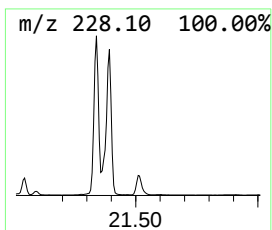
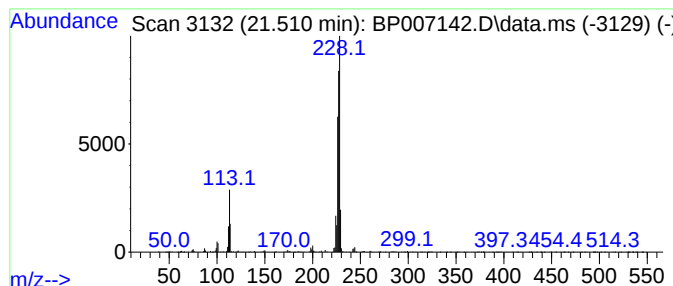
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclopenta(cd)pyrene, 3,4-d... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.510	2.25 ng	1132460	Chrysene-d12	21.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	95
2			Benzo[c]phenanthrene	228	C18H12	000195-19-7	58
3			5-Phenylthieno[2,3-d]pyrimidin-4-ol	228	C12H8N2O5	035978-39-3	52
4			Dimethyl-[4-[2-(3-methylisoxazol...	228	C14H16N2O	1000306-39-6	50
5			Triphenylene	228	C18H12	000217-59-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092321\
Data File : BP007142.D
Acq On : 24 Sep 2021 01:01
Operator : CG/JU
Sample : M3797-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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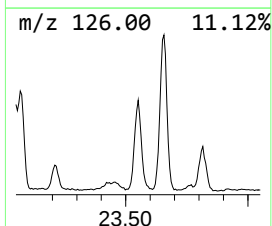
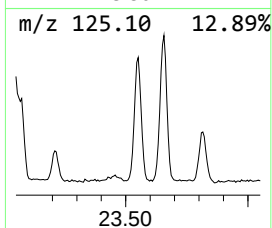
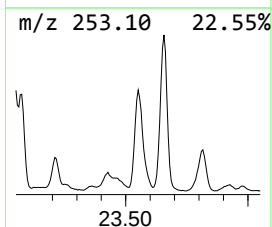
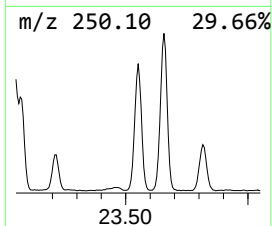
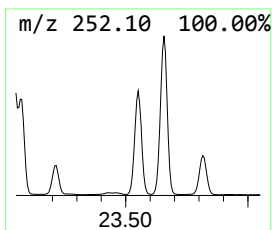
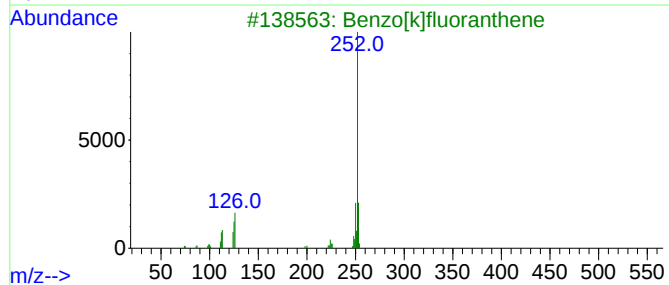
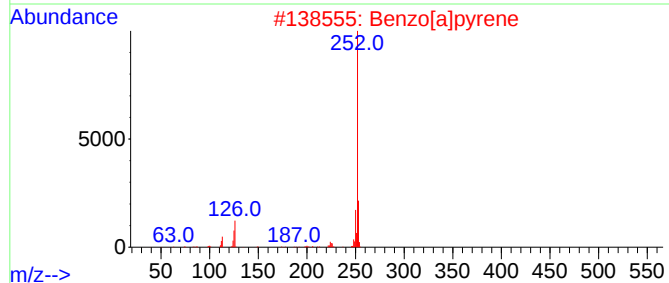
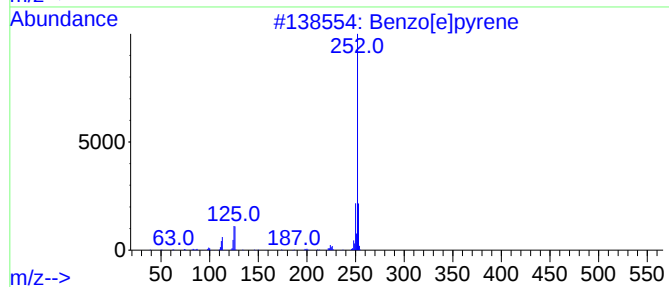
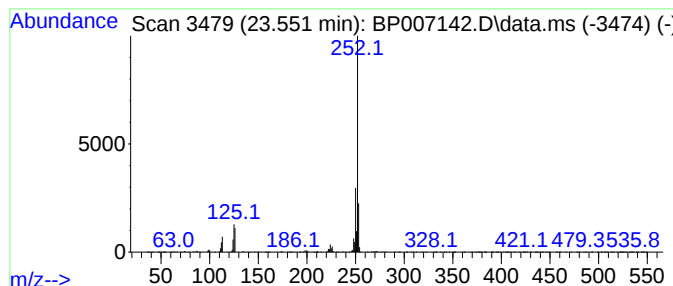
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.551	22.17 ng	3627320	Perylene-d12	23.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[a]pyrene	252	C20H12	000050-32-8	98
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5			Perylene	252	C20H12	000198-55-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092321\
Data File : BP007142.D
Acq On : 24 Sep 2021 01:01
Operator : CG/JU
Sample : M3797-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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Phenol, 2,6-bis...	13.869	5.0	ng	994719	3	14.522	3939180	20.0
unknown14.351	14.351	3.0	ng	580231	3	14.522	3939180	20.0
unknown15.310	15.310	2.1	ng	404962	3	14.522	3939180	20.0
Pentadecane, 2,...	16.263	9.4	ng	1782150	4	17.269	3781840	20.0
Hexadecane, 2,6...	17.086	17.5	ng	3313050	4	17.269	3781840	20.0
11H-Benzo[b]flu...	20.110	4.0	ng	1991540	5	21.357	10049600	20.0
11H-Benzo[a]flu...	20.210	2.7	ng	1374940	5	21.357	10049600	20.0
Cyclopenta(cd)p...	21.510	2.3	ng	1132460	5	21.357	10049600	20.0
Benzo[e]pyrene	23.551	22.2	ng	3627320	6	23.762	3272420	20.0