

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
 Data File : BP019836.D
 Acq On : 22 Feb 2024 21:46
 Operator : MA/JU
 Sample : P1537-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 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_P\Methods\8270E-BP013124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019836.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.128	3	7	19	rVB	790028	949804	27.50%	3.622%
2	4.070	161	167	176	rVB3	51976	91546	2.65%	0.349%
3	4.640	259	264	269	rBV	94212	134203	3.89%	0.512%
4	4.693	269	273	279	rVB	50461	71891	2.08%	0.274%
5	5.017	320	328	339	rBV	211627	314954	9.12%	1.201%
6	5.470	398	405	415	rBV	872983	1355304	39.24%	5.168%
7	7.069	668	677	692	rBV	796928	1351201	39.12%	5.152%
8	7.893	811	817	824	rVB	282754	462584	13.39%	1.764%
9	9.063	1008	1016	1029	rBV	498006	885106	25.63%	3.375%
10	10.693	1285	1293	1305	rBV	338528	599702	17.36%	2.287%
11	13.157	1704	1712	1729	rBV	1291648	2058558	59.61%	7.849%
12	14.257	1894	1899	1907	rVB	24689	45949	1.33%	0.175%
13	14.528	1933	1945	1952	rBV	538025	859730	24.89%	3.278%
14	16.028	2190	2200	2212	rBV	1309967	2026153	58.67%	7.726%
15	17.292	2408	2415	2419	rBV	732319	1118761	32.39%	4.266%
16	17.334	2419	2422	2430	rVV	319839	441202	12.77%	1.682%
17	17.422	2433	2437	2443	rVB	59943	91478	2.65%	0.349%
18	18.186	2563	2567	2576	rVB2	219839	384142	11.12%	1.465%
19	18.345	2589	2594	2598	rBV3	83685	141525	4.10%	0.540%
20	18.381	2598	2600	2607	rVB	43729	50308	1.46%	0.192%
21	18.645	2641	2645	2648	rBV	39032	50314	1.46%	0.192%
22	18.692	2648	2653	2660	rVB2	65670	98732	2.86%	0.376%
23	19.045	2709	2713	2717	rBV	42033	66935	1.94%	0.255%
24	19.181	2733	2736	2742	rBV2	43546	72770	2.11%	0.277%
25	19.298	2751	2756	2765	rBV	1022957	1463341	42.37%	5.580%
26	19.422	2774	2777	2780	rBV2	52943	61310	1.78%	0.234%
27	19.651	2812	2816	2825	rVB	871830	1250215	36.20%	4.767%
28	19.857	2845	2851	2864	rVB	2734714	3453645	100.00%	13.169%
29	19.975	2867	2871	2876	rVB4	51836	105058	3.04%	0.401%
30	20.139	2896	2899	2903	rVB	93929	109356	3.17%	0.417%
31	20.239	2913	2916	2920	rVB	57621	67654	1.96%	0.258%
32	21.069	3055	3057	3060	rBV	60138	70432	2.04%	0.269%
33	21.104	3060	3063	3069	rVB3	258373	333853	9.67%	1.273%
34	21.380	3104	3110	3114	rBV2	1061380	1962330	56.82%	7.482%
35	21.422	3114	3117	3126	rVB	479981	671508	19.44%	2.560%
36	21.545	3135	3138	3144	rVB	92696	121269	3.51%	0.462%

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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-BP013124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.069	3392	3397	3403	rBV	426053	1029992	29.82%	3.927%
38	23.698	3499	3504	3514	rVB	352324	734487	21.27%	2.801%
39	23.804	3517	3522	3529	rVV	537702	1068585	30.94%	4.075%

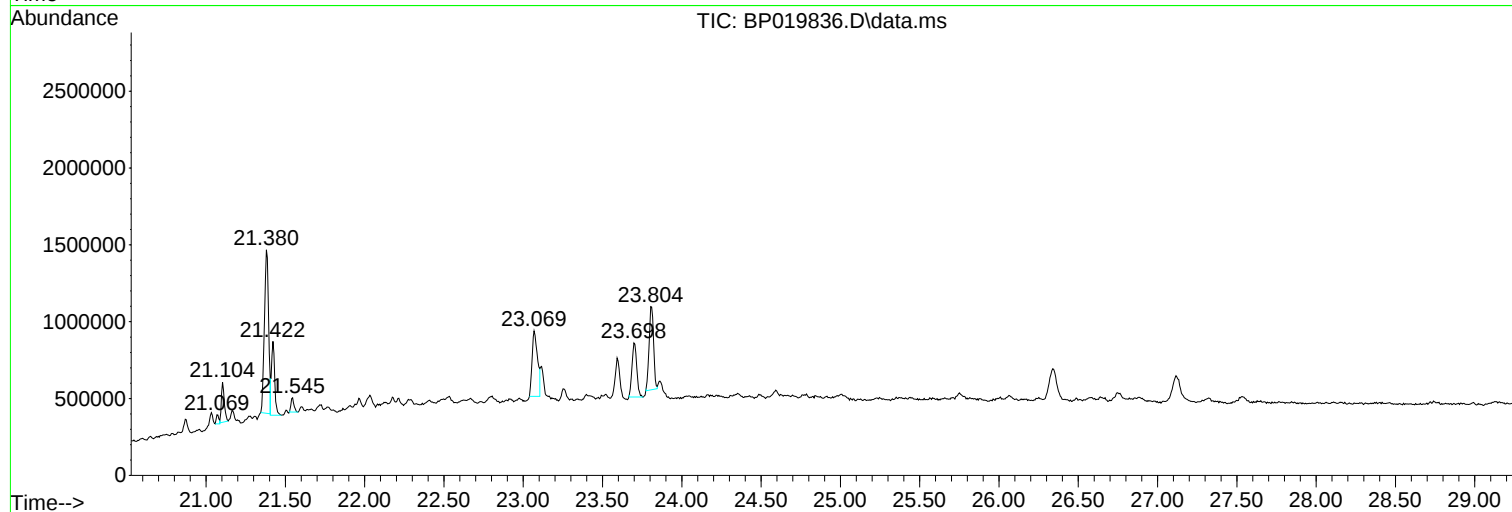
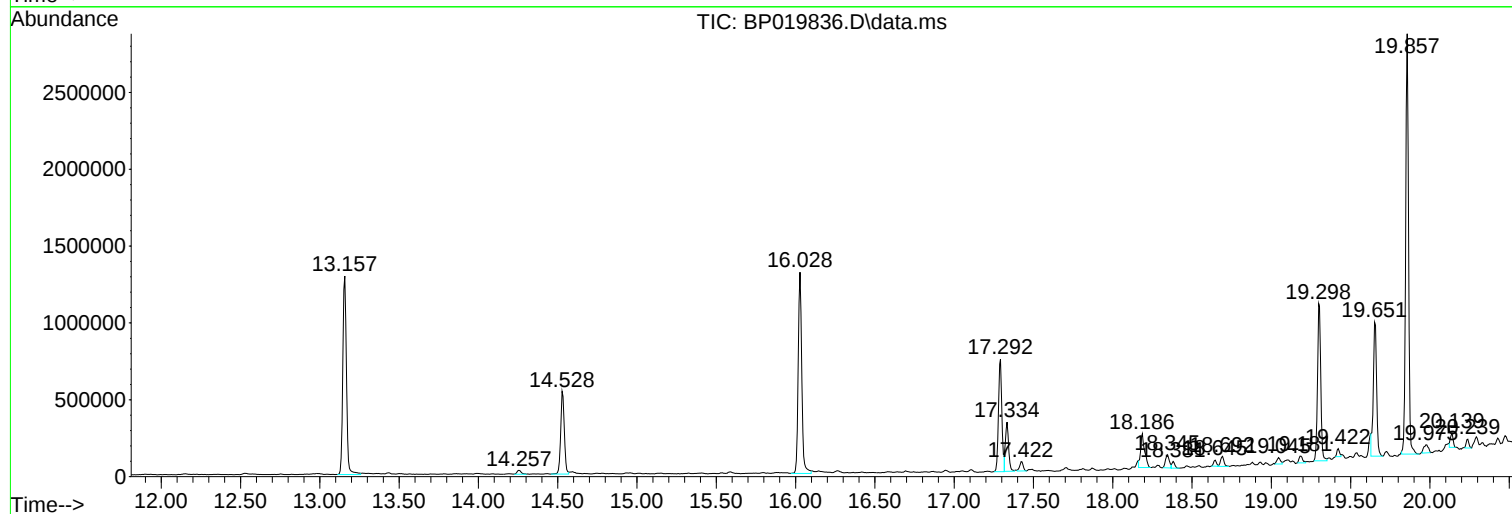
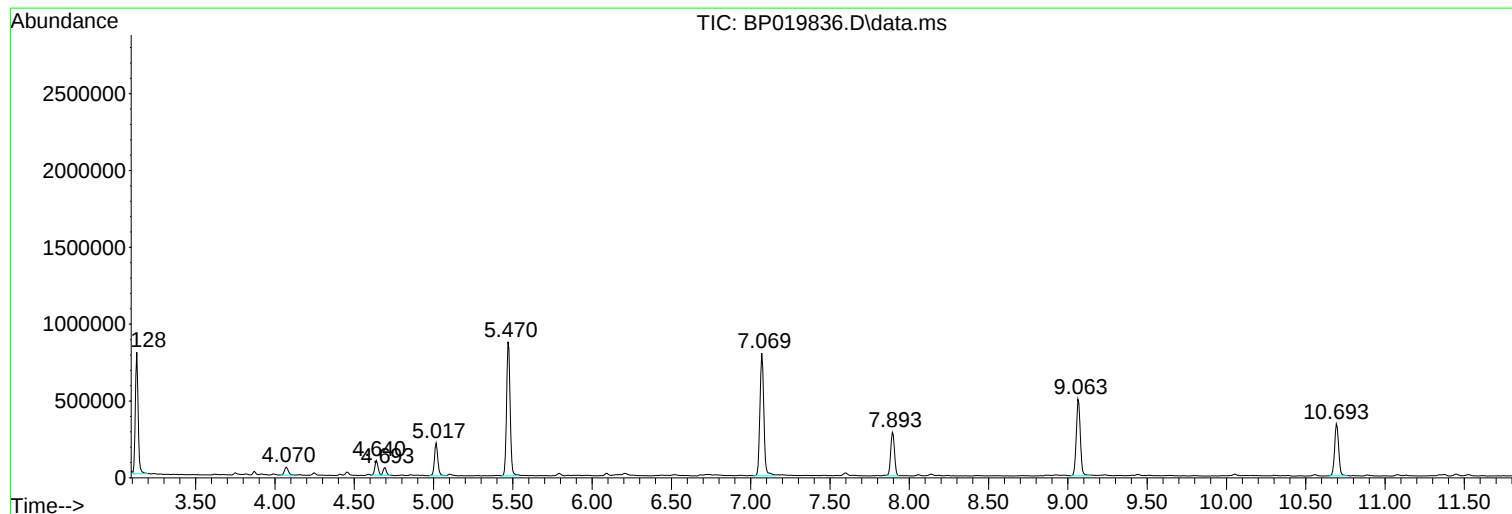
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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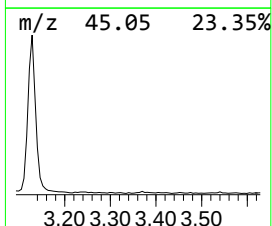
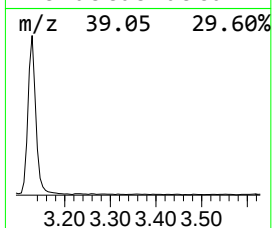
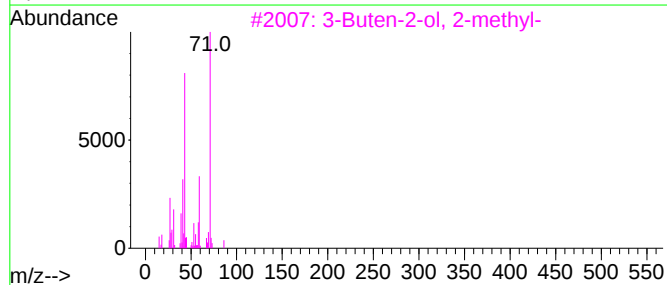
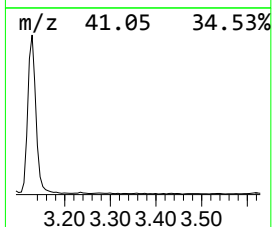
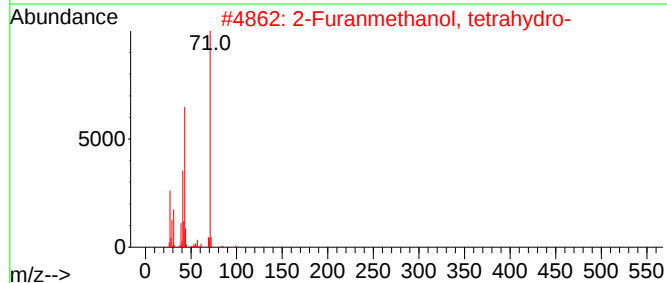
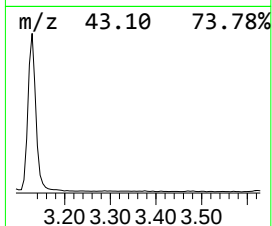
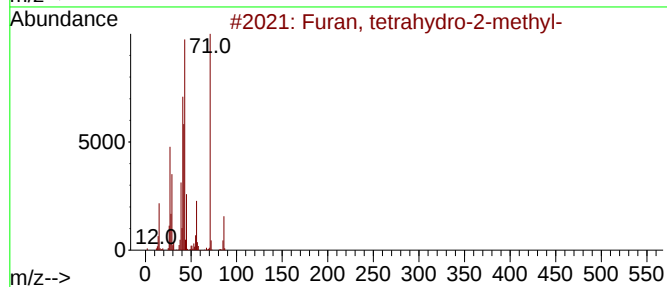
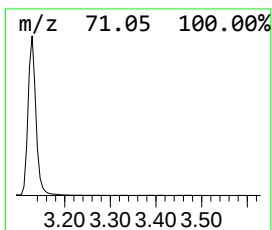
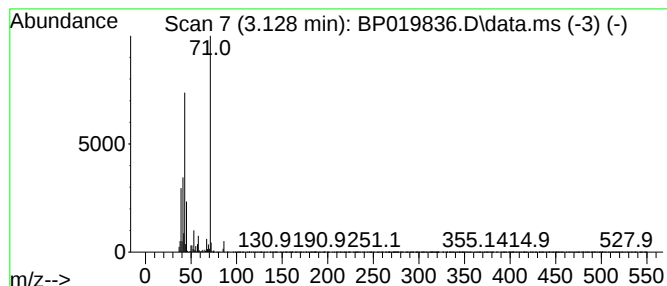
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Furan, tetrahydro-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	41.07 ng	949804	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	50
2			2-Furanmethanol, tetrahydro-	102	C5H10O2	000097-99-4	50
3			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	50
4			3-Penten-2-ol	86	C5H10O	001569-50-2	47
5			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	45



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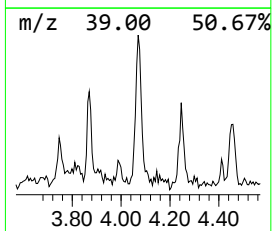
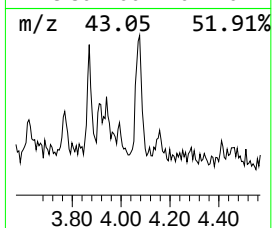
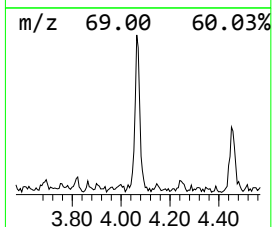
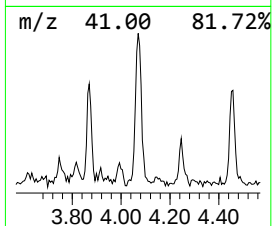
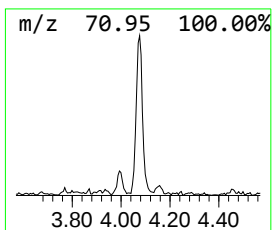
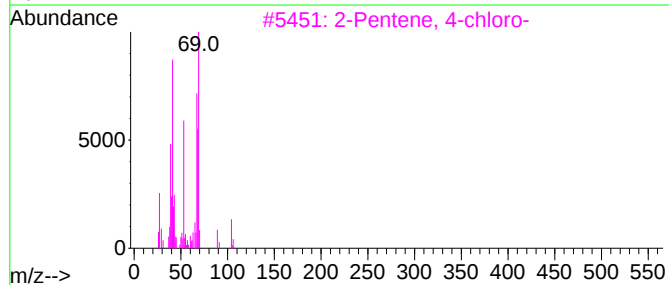
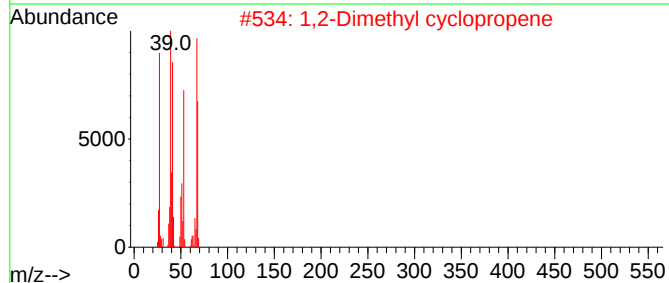
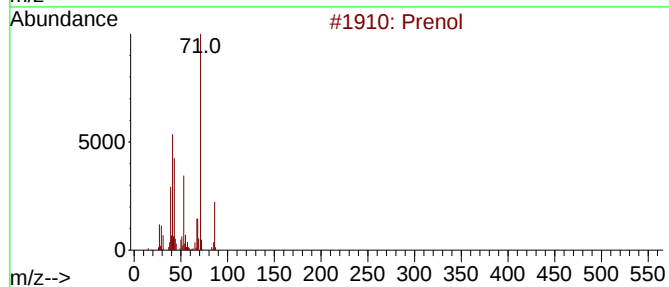
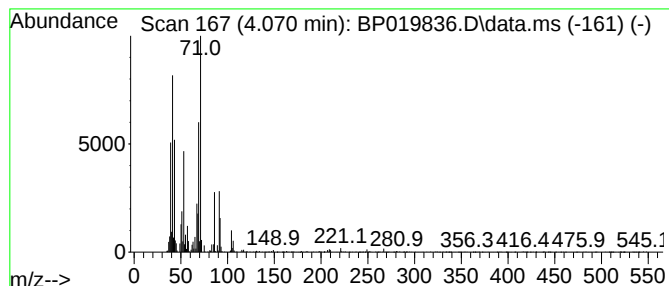
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Prenol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.070	3.96 ng	91546	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prenol	86	C5H10O	000556-82-1	64
2	1,2-Dimethyl cyclopropene	68	C5H8	014309-32-1	52
3	2-Pentene, 4-chloro-	104	C5H9Cl	001458-99-7	32
4	1-Butene, 1-chloro-3-methyl-	104	C5H9Cl	023010-00-6	32
5	2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	27



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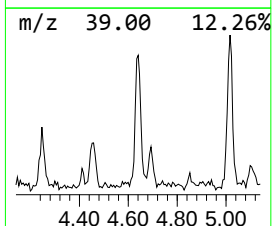
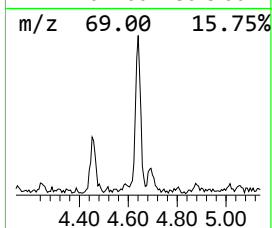
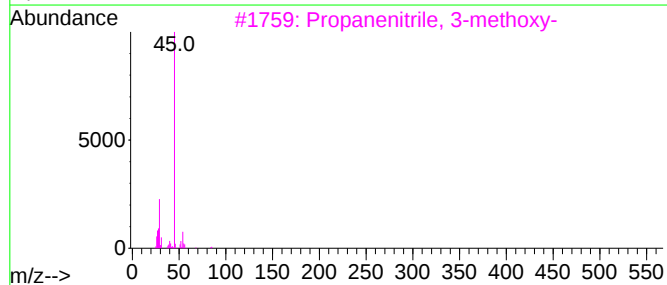
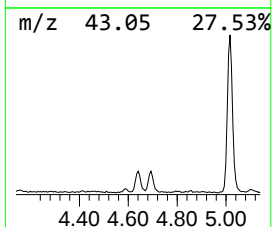
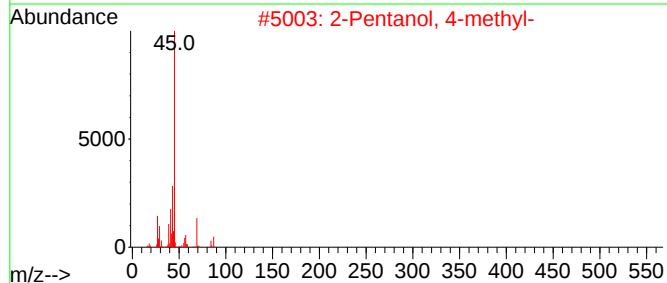
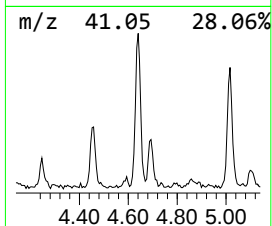
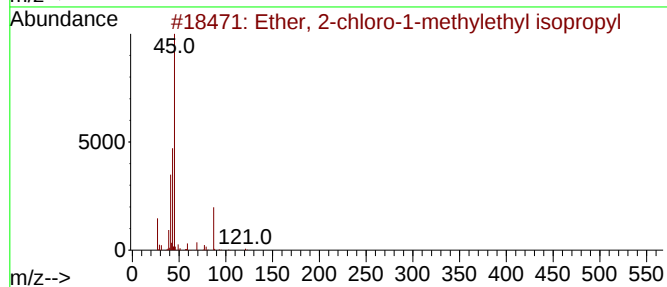
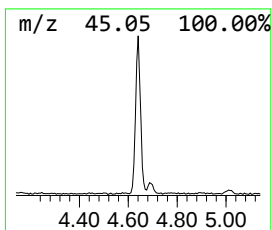
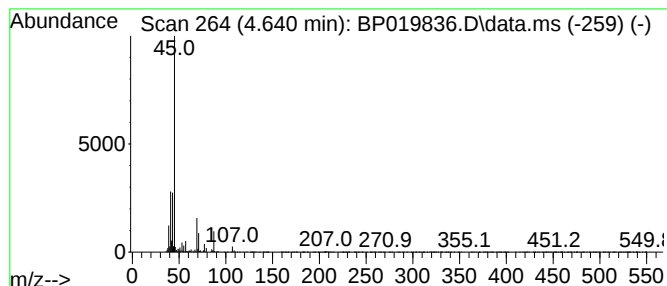
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ether, 2-chloro-1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.640	5.80 ng	134203	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ether, 2-chloro-1-methylethyl is...	136	C6H13ClO	098277-76-0	64
2			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	59
3			Propanenitrile, 3-methoxy-	85	C4H7NO	000110-67-8	42
4			2-Hexanol	102	C6H14O	000626-93-7	39
5			Hexane, 1-methoxy-	116	C7H16O	004747-07-3	38



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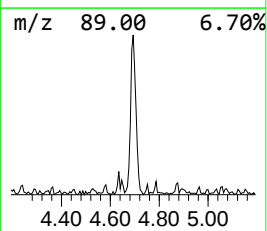
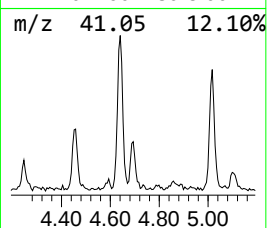
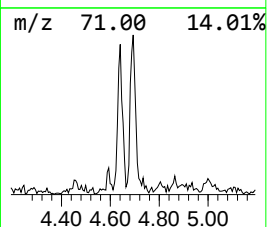
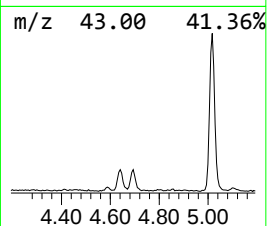
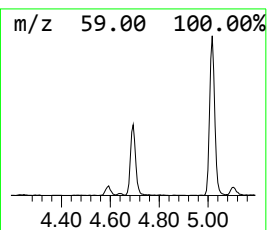
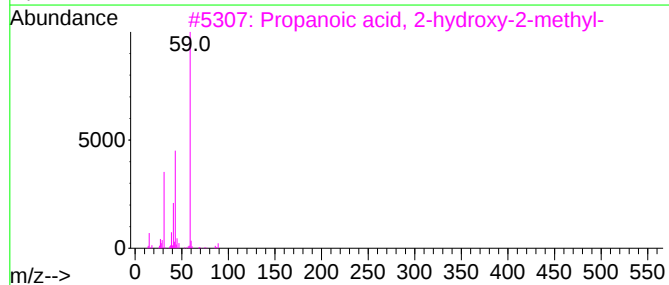
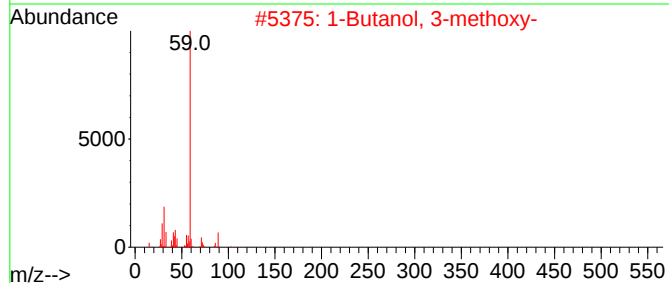
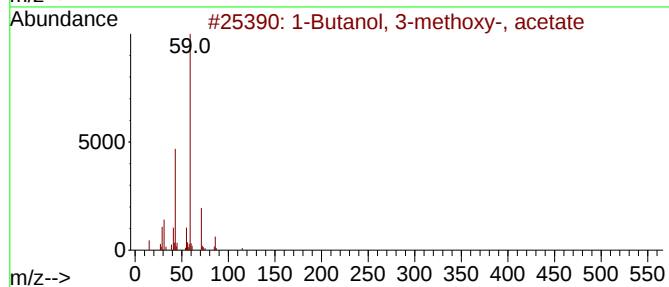
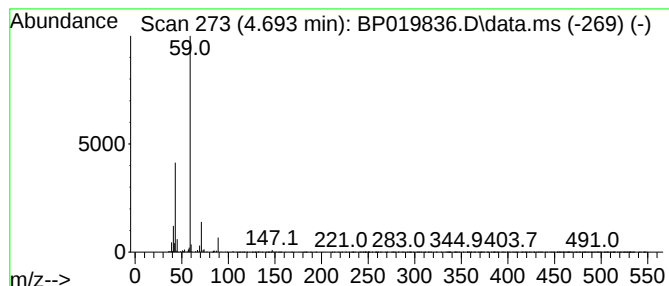
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Butanol, 3-methoxy-, acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.693	3.11 ng	71891	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 3-methoxy-, acetate	146	C7H14O3	004435-53-4	56		
2	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	56		
3	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	39		
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	9		
5	2-Propanol, 1-(isooctyloxy)-2-me...	202	C12H26O2	056282-27-0	9		



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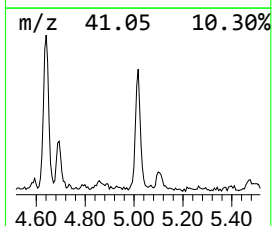
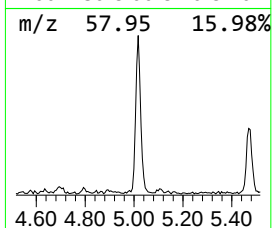
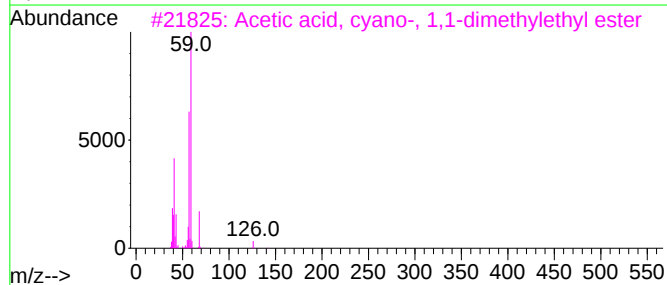
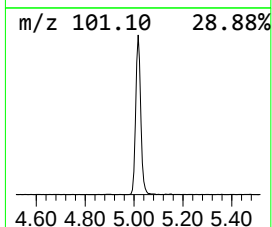
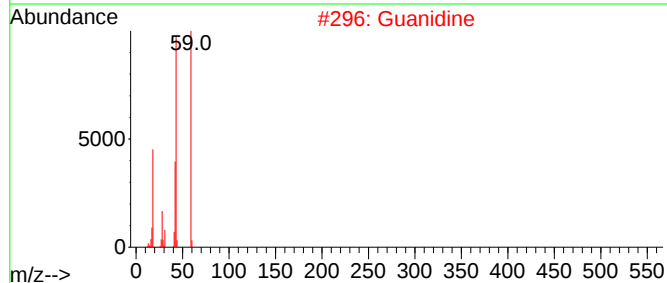
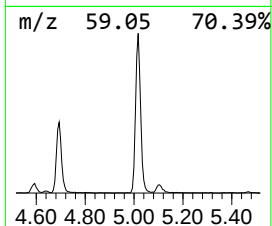
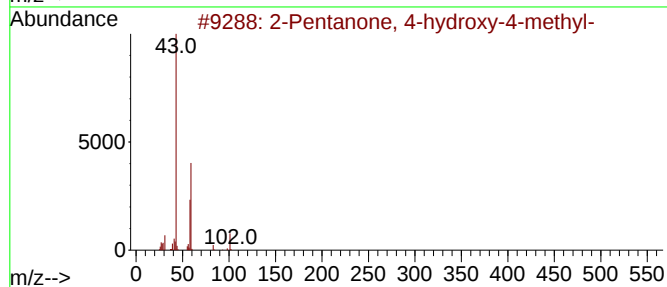
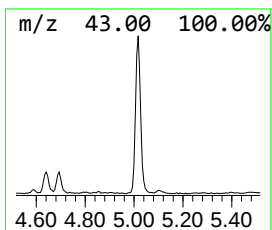
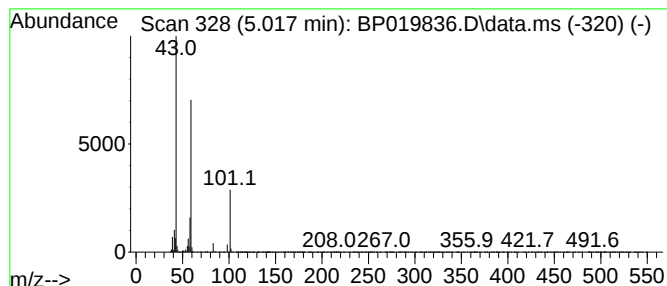
Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.017	13.62 ng	314954	1,4-Dichlorobenzene-d4	7.893	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Guanidine	59	CH5N3	000113-00-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019836.D
Acq On : 22 Feb 2024 21:46
Operator : MA/JU
Sample : P1537-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

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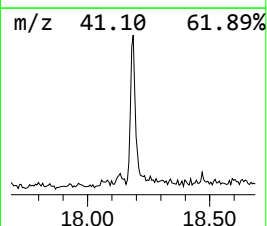
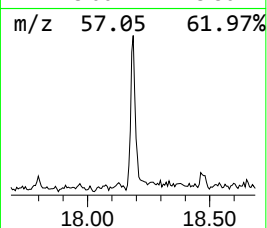
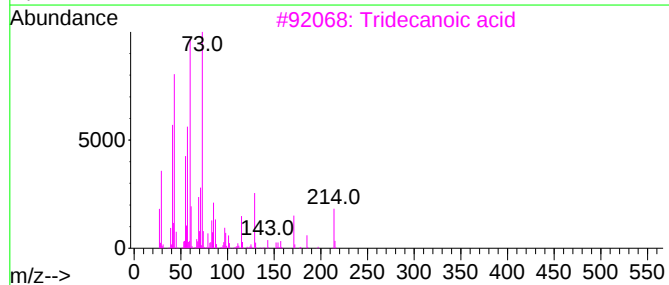
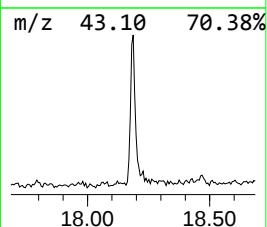
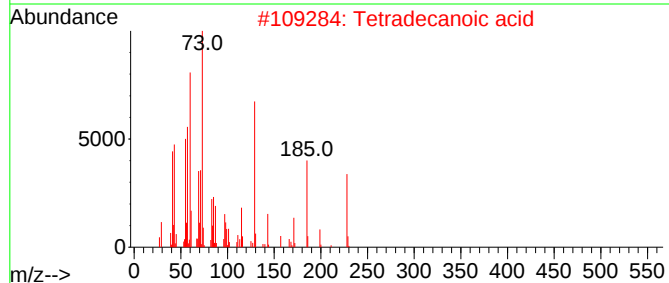
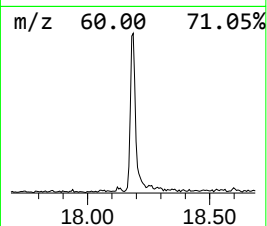
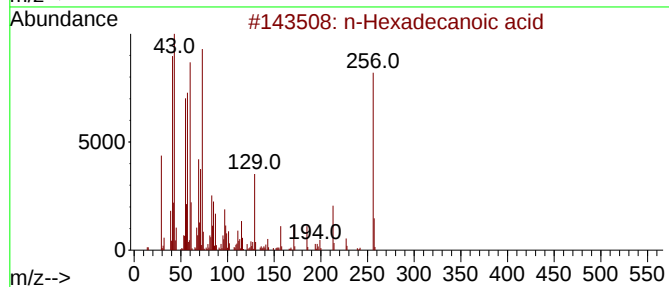
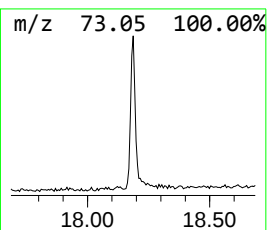
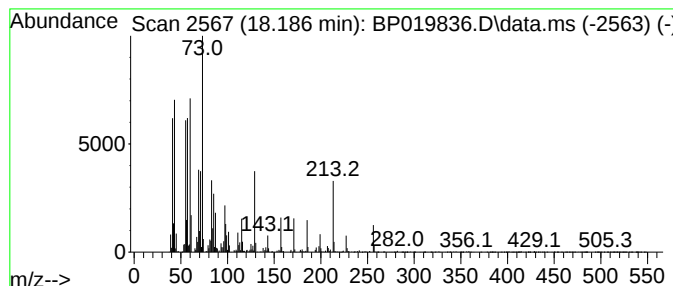
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	6.87 ng	384142	Phenanthrene-d10	17.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	58
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5		Octadecanoic acid	284	C18H36O2	000057-11-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019836.D
Acq On : 22 Feb 2024 21:46
Operator : MA/JU
Sample : P1537-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

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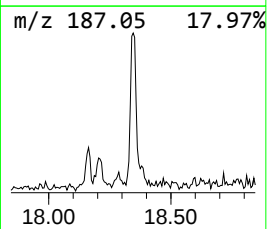
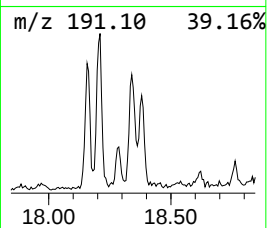
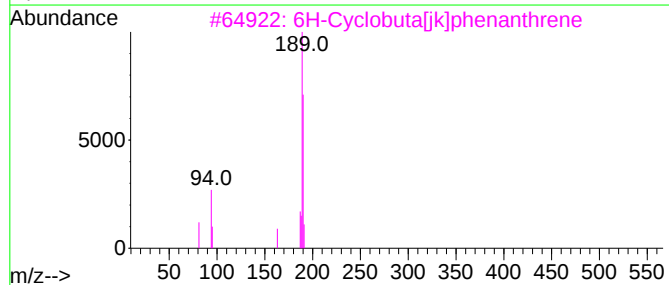
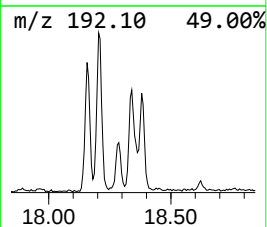
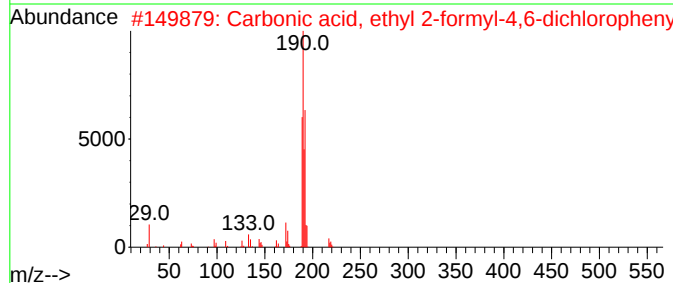
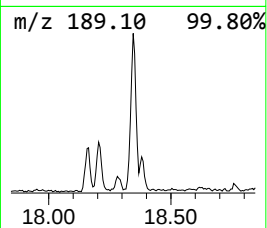
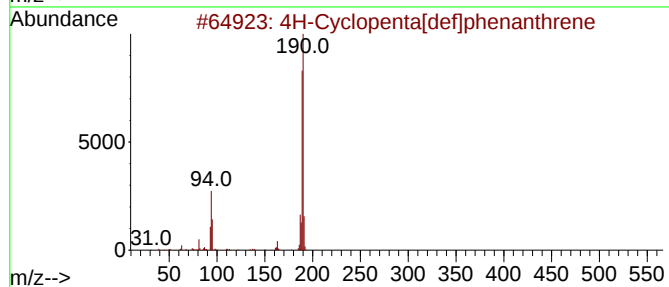
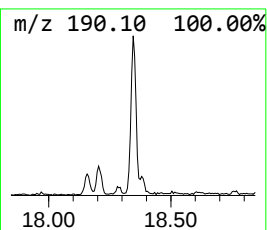
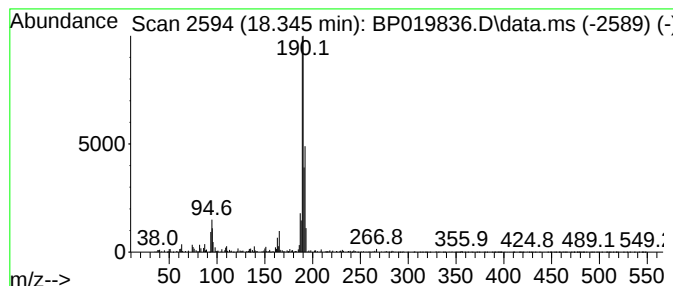
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	2.53 ng	141525	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2			Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	53
3			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
4			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43
5			1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
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Acq On : 22 Feb 2024 21:46
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Sample : P1537-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
1

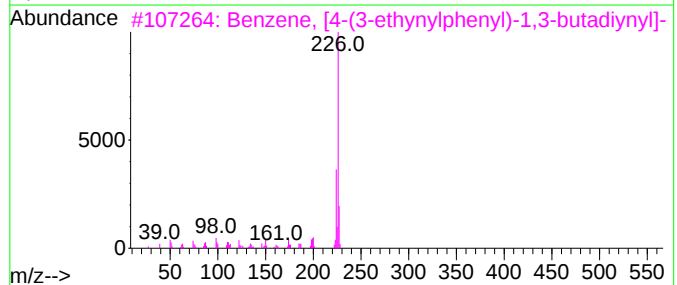
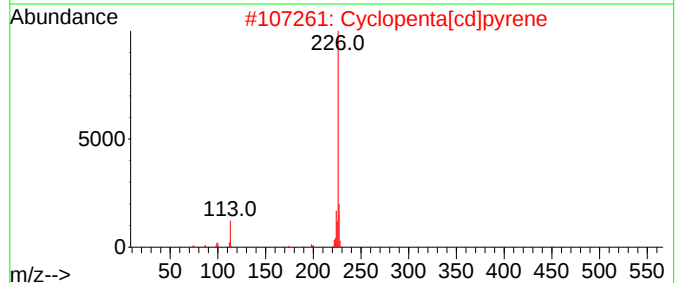
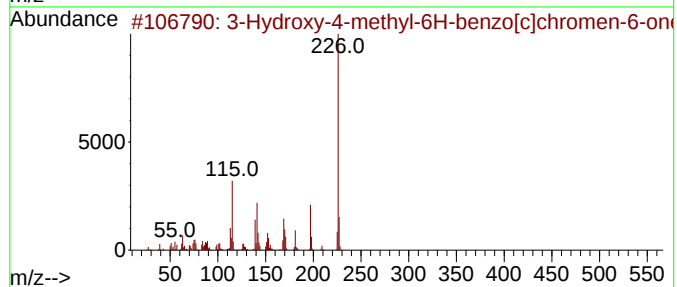
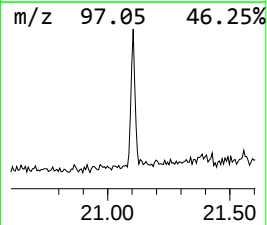
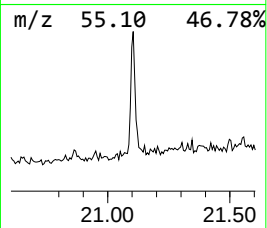
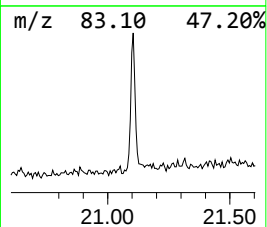
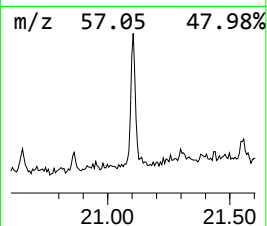
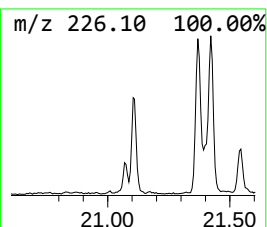
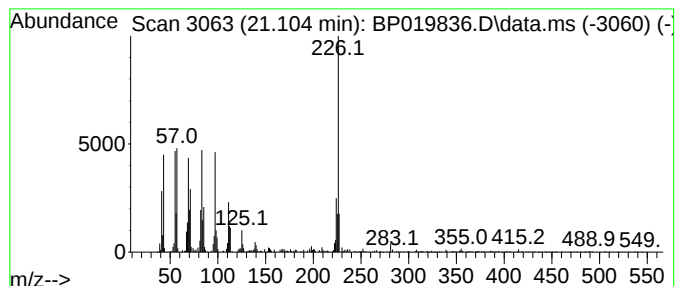
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown21.104 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.104	3.40 ng	333853	Chrysene-d12	21.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hydroxy-4-methyl-6H-benzo[c]ch...	226	C14H10O3	076244-77-4	25
2			Cyclopenta[cd]pyrene	226	C18H10	027208-37-3	25
3			Benzene, [4-(3-ethynylphenyl)-1,...	226	C18H10	1000115-87-3	22
4			Anthralin	226	C14H10O3	001143-38-0	22
5			Pentanedioic acid, 1-(6-bromo-9-...	625	C35H48BrNO4	049646-95-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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
Furan, tetrahyd...	3.128	41.1	ng	949804	1	7.893	462584	20.0
Prenol	4.070	4.0	ng	91546	1	7.893	462584	20.0
Ether, 2-chloro...	4.640	5.8	ng	134203	1	7.893	462584	20.0
1-Butanol, 3-me...	4.693	3.1	ng	71891	1	7.893	462584	20.0
2-Pentanone, 4-...	5.017	13.6	ng	314954	1	7.893	462584	20.0
n-Hexadecanoic ...	18.186	6.9	ng	384142	4	17.292	1118760	20.0
4H-Cyclopenta[d]...	18.345	2.5	ng	141525	4	17.292	1118760	20.0
unknown21.104	21.104	3.4	ng	333853	5	21.386	1962330	20.0