

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021424\
 Data File : BP019706.D
 Acq On : 14 Feb 2024 17:47
 Operator : MA/JU
 Sample : P1449-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 ETGI-362

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: BP019706.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.628	88	92	107	rBV	72907	112249	2.92%	0.416%
2	5.481	400	407	417	rBV	911948	1395136	36.27%	5.176%
3	7.075	669	678	694	rBV	886658	1469749	38.21%	5.453%
4	7.904	811	819	826	rBV	274352	446496	11.61%	1.656%
5	9.069	1008	1017	1029	rBV	566549	969654	25.21%	3.597%
6	10.704	1285	1295	1302	rBV	332230	590675	15.36%	2.191%
7	11.457	1417	1423	1431	rBV2	37338	71573	1.86%	0.266%
8	13.163	1706	1713	1732	rBV	1519663	2320428	60.33%	8.609%
9	14.533	1938	1946	1954	rBV	522132	823036	21.40%	3.053%
10	14.763	1983	1985	1994	rVB	1050770	1405815	36.55%	5.215%
11	16.027	2191	2200	2219	rBV	1404517	2259593	58.75%	8.383%
12	17.292	2406	2415	2419	rBV	728096	1067560	27.76%	3.961%
13	17.333	2419	2422	2429	rVV	294065	418313	10.88%	1.552%
14	17.427	2433	2438	2443	rVB	49024	75658	1.97%	0.281%
15	17.704	2474	2485	2497	rBV2	27494	79035	2.05%	0.293%
16	18.163	2555	2563	2564	rBV	43745	64909	1.69%	0.241%
17	18.192	2564	2568	2576	rVB2	273991	443422	11.53%	1.645%
18	18.345	2589	2594	2598	rBV2	85532	136175	3.54%	0.505%
19	18.380	2598	2600	2607	rVB	35020	48052	1.25%	0.178%
20	18.645	2641	2645	2649	rBV	37407	51371	1.34%	0.191%
21	18.686	2649	2652	2657	rVB	56141	75642	1.97%	0.281%
22	19.045	2709	2713	2717	rBV2	23297	38594	1.00%	0.143%
23	19.110	2719	2724	2727	rVV6	30648	41730	1.08%	0.155%
24	19.186	2732	2737	2743	rBV2	30886	53606	1.39%	0.199%
25	19.304	2750	2757	2766	rBV	803263	1141372	29.67%	4.234%
26	19.427	2774	2778	2785	rVB3	79630	117434	3.05%	0.436%
27	19.627	2807	2812	2813	rBV2	143070	190289	4.95%	0.706%
28	19.657	2813	2817	2825	rVV	649423	919337	23.90%	3.411%
29	19.721	2825	2828	2834	rVB3	31599	48863	1.27%	0.181%
30	19.857	2842	2851	2864	rBV	2867122	3846242	100.00%	14.269%
31	19.968	2865	2870	2877	rVV3	43946	108867	2.83%	0.404%
32	20.104	2888	2893	2895	rBV4	42239	72150	1.88%	0.268%
33	20.139	2895	2899	2903	rVB	112508	149666	3.89%	0.555%
34	20.239	2911	2916	2919	rBV	85666	115792	3.01%	0.430%
35	20.292	2920	2925	2929	rVB2	54002	89476	2.33%	0.332%
36	20.474	2953	2956	2960	rVB2	31166	45656	1.19%	0.169%

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Instrument :
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ClientSampleId :
ETGI-362

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	20.868	3020	3023	3029	rVB	54420	73504	1.91%	0.273%
38	21.033	3047	3051	3055	rBV2	58960	88002	2.29%	0.326%
39	21.074	3055	3058	3060	rVV	60999	69401	1.80%	0.257%
40	21.109	3060	3064	3069	rVV2	280531	380221	9.89%	1.411%
41	21.162	3070	3073	3079	rVB	66014	89955	2.34%	0.334%
42	21.386	3104	3111	3114	rBV2	1004603	1768392	45.98%	6.561%
43	21.421	3114	3117	3125	rVB	374471	530509	13.79%	1.968%
44	21.545	3135	3138	3144	rVB3	47697	85835	2.23%	0.318%
45	23.062	3391	3396	3401	rBV	288136	653686	17.00%	2.425%
46	23.586	3481	3485	3495	rVB	171739	346110	9.00%	1.284%
47	23.692	3498	3503	3510	rVB	230682	443970	11.54%	1.647%
48	23.798	3515	3521	3528	rBV	545820	1121700	29.16%	4.161%

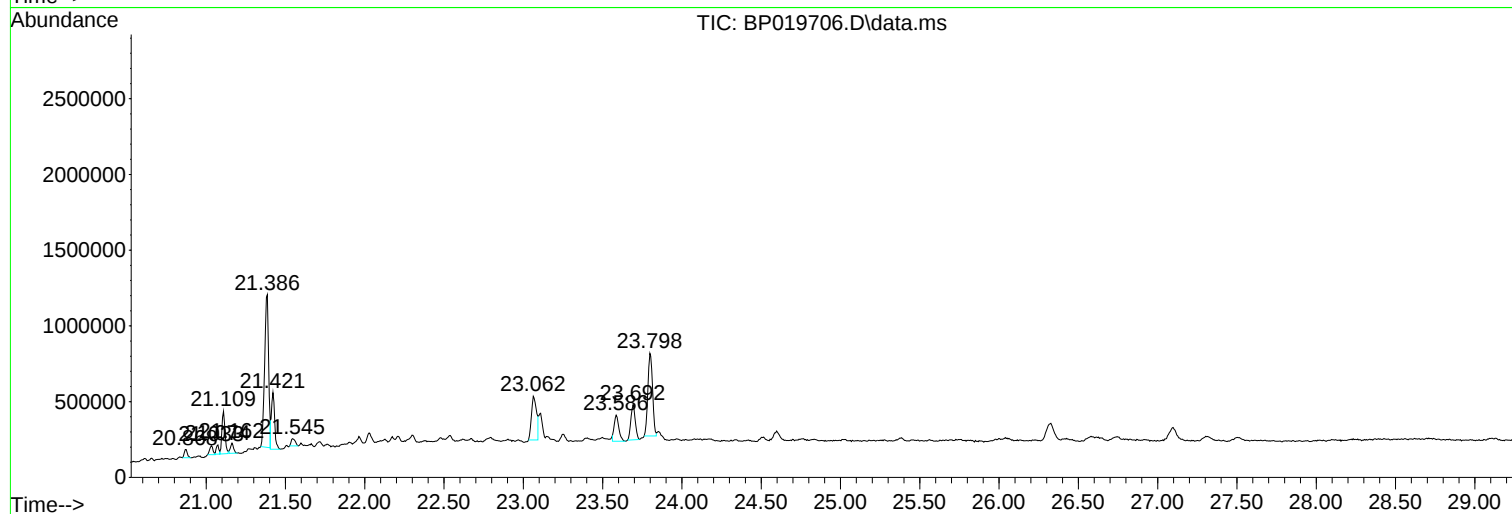
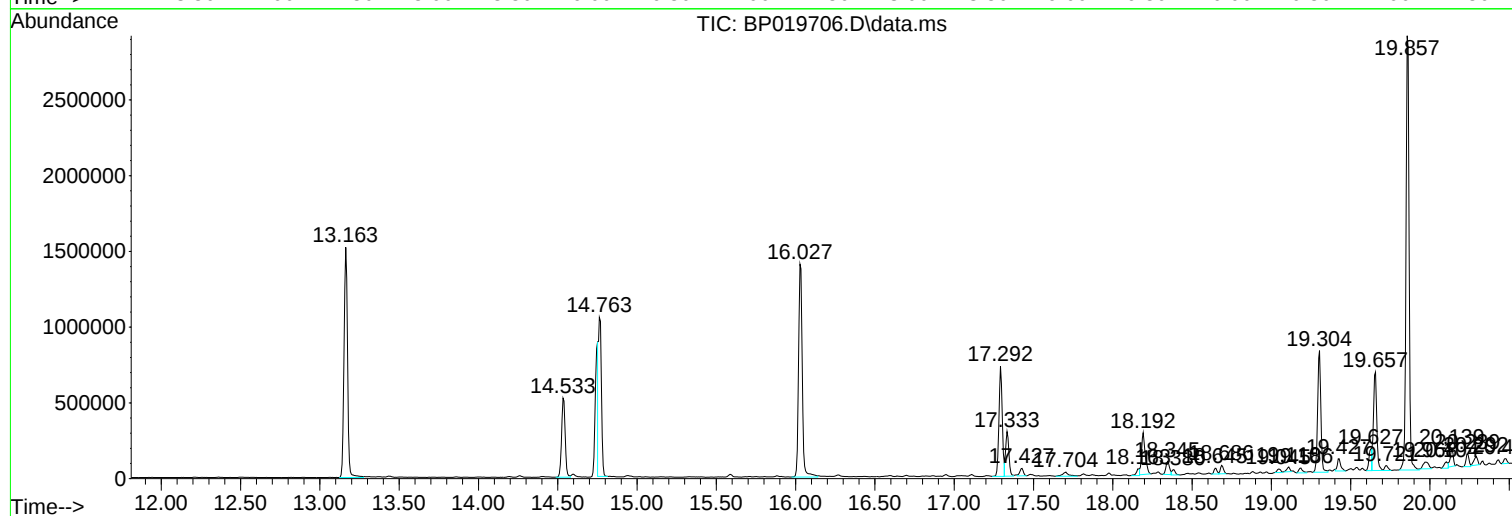
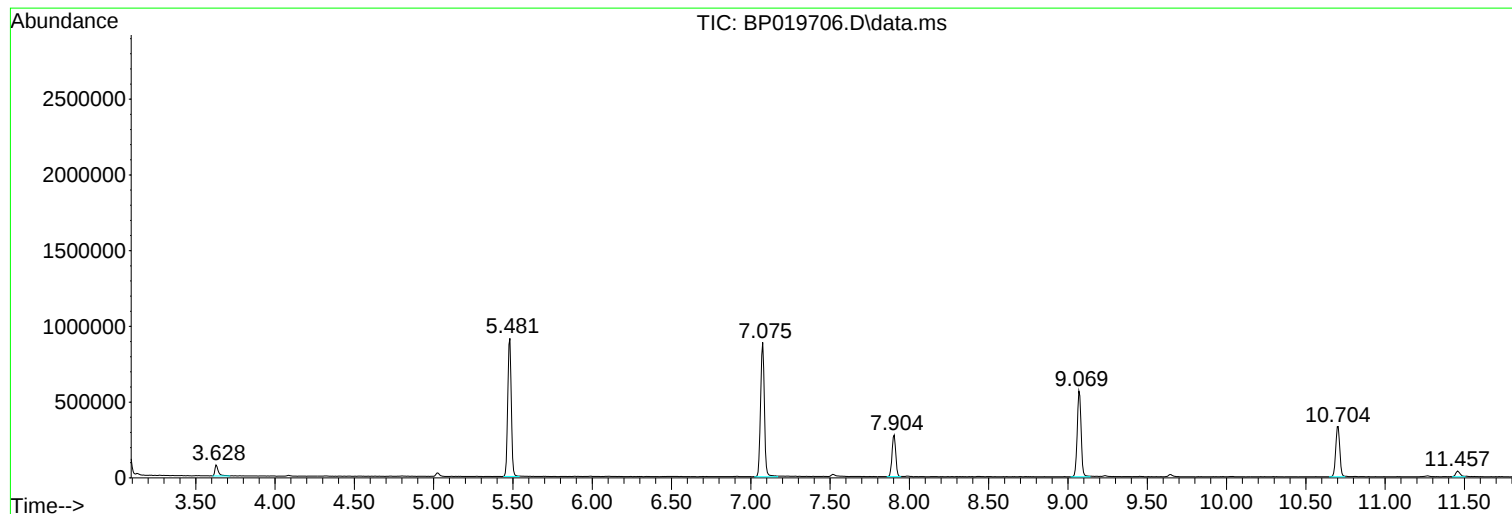
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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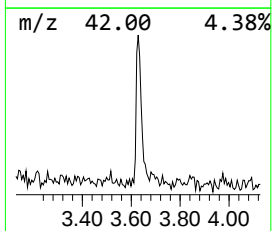
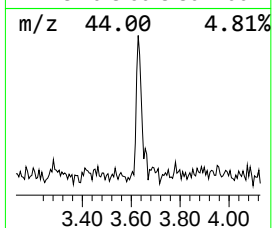
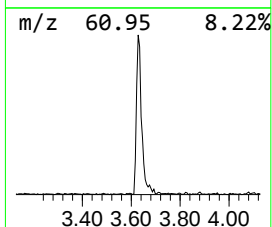
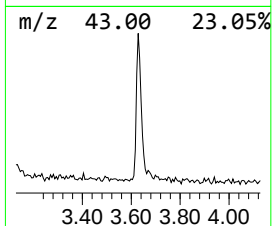
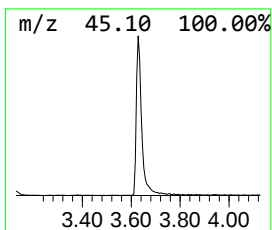
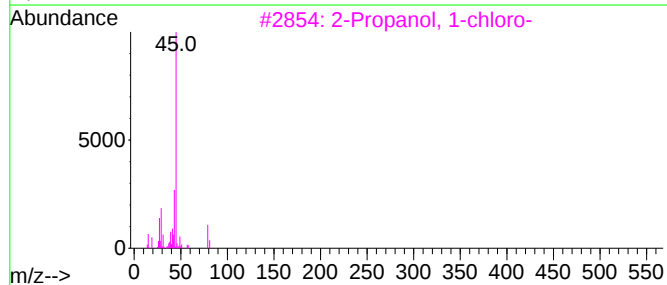
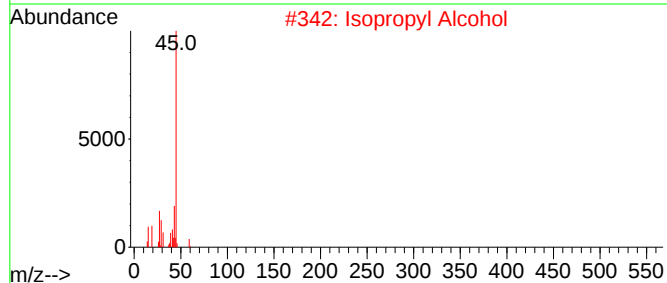
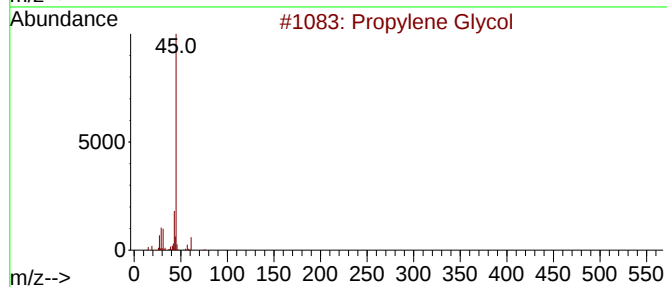
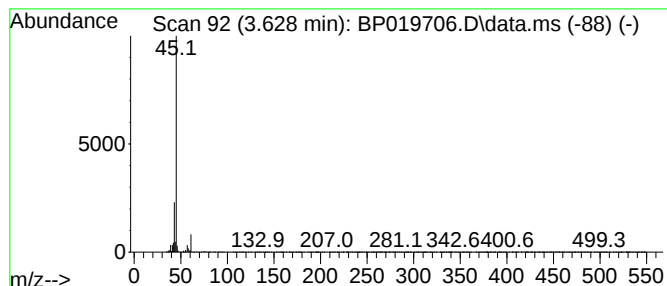
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.628	5.03 ng	112249	1,4-Dichlorobenzene-d4	7.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	78
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			2-Propanol, 1-chloro-	94	C3H7ClO	000127-00-4	40
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			2-Hexanol	102	C6H14O	000626-93-7	9



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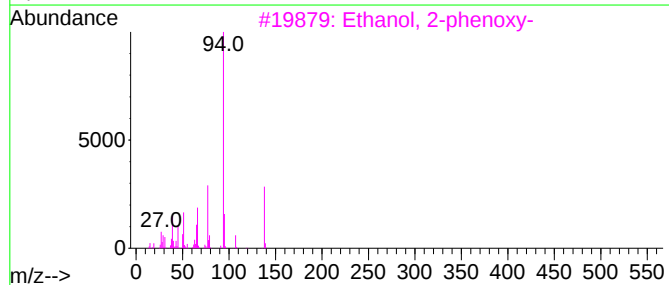
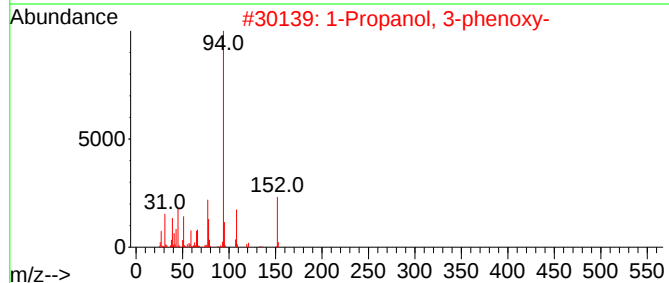
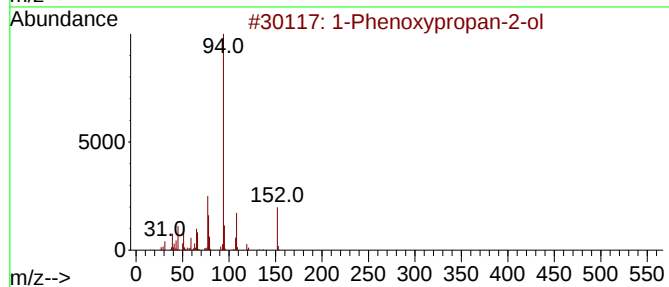
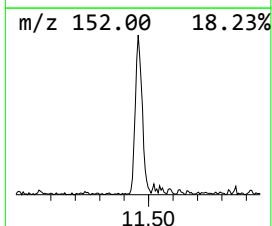
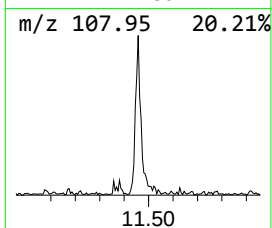
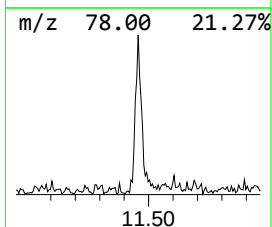
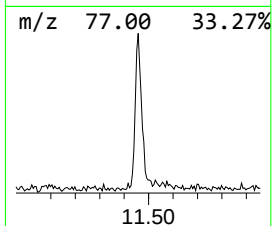
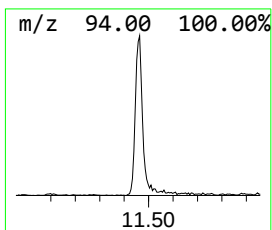
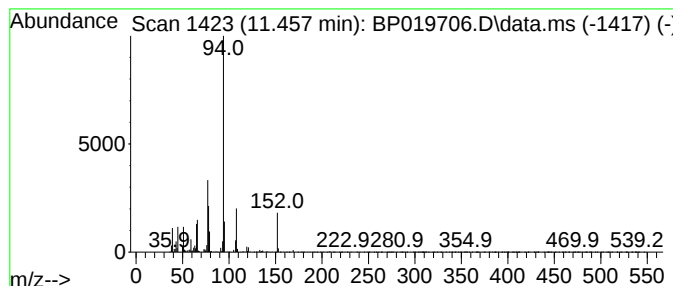
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.457	2.42 ng	71573	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	74
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
4			1-Amino-3-phenoxypropan-2-ol	167	C9H13NO2	004287-19-8	53
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	50



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ALS Vial : 15 Sample Multiplier: 1

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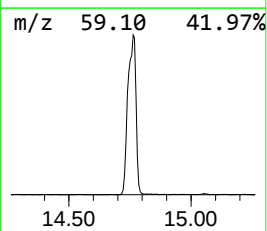
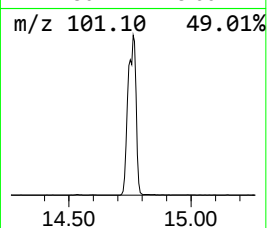
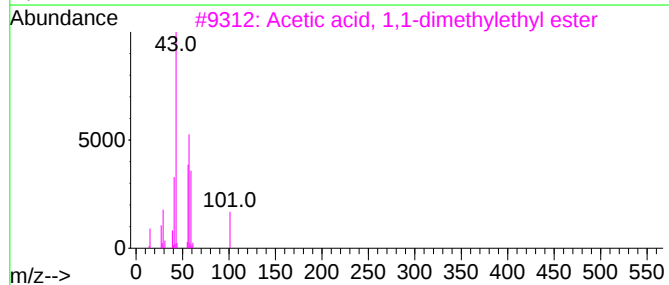
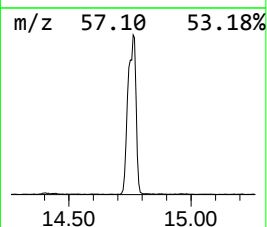
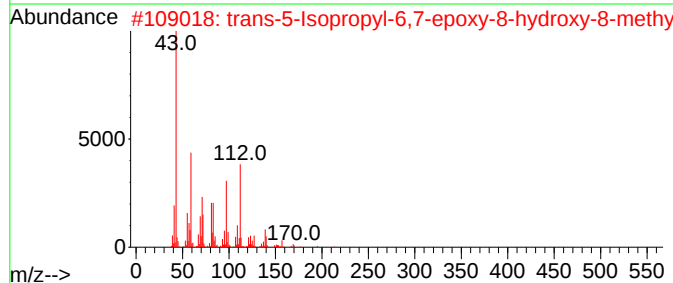
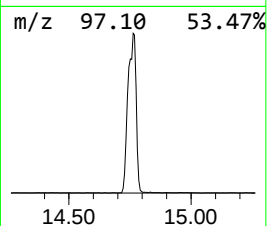
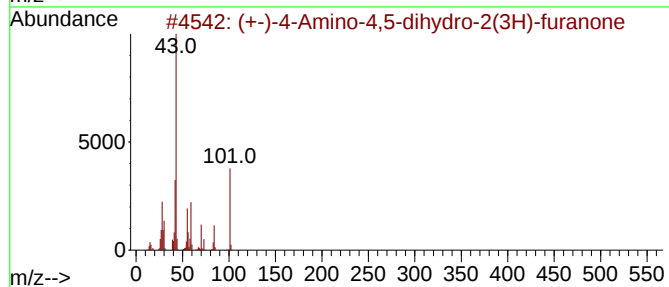
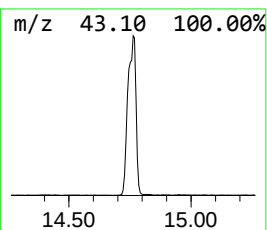
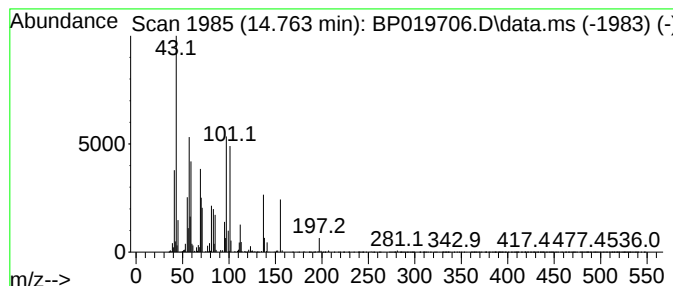
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown14.763 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	34.16 ng	1405820	Acenaphthene-d10	14.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	27		
2	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	25		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	22		
4	7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	14		
5	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	10		



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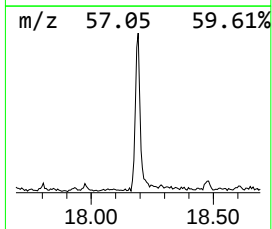
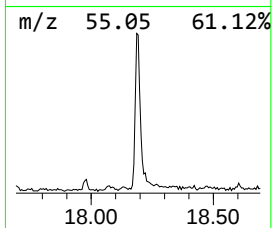
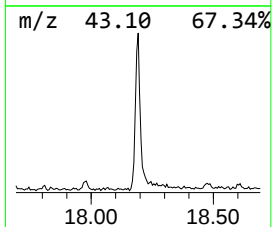
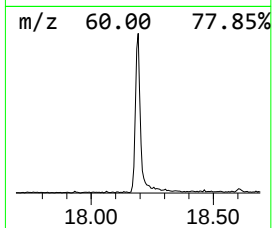
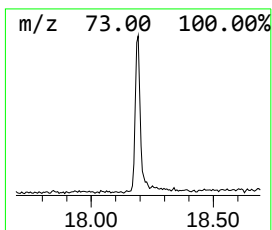
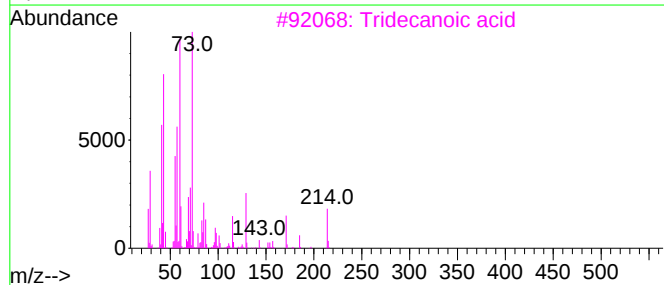
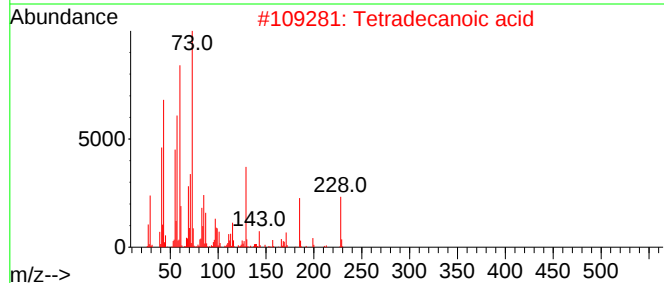
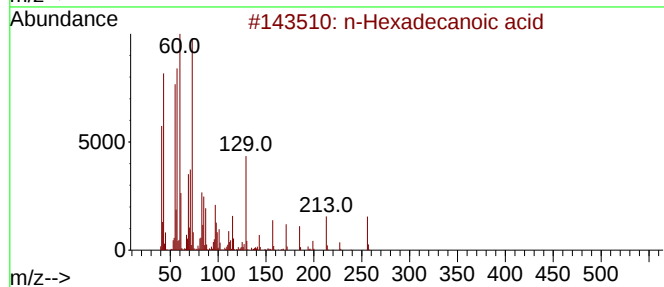
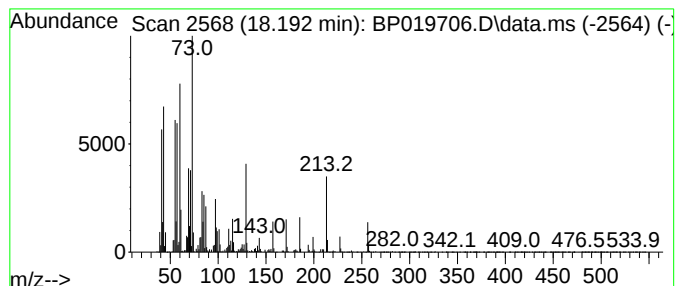
Instrument :
BNA_P
ClientSampleId :
ETGI-362

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 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.192	8.31 ng	443422	Phenanthrene-d10	17.292	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Octadecanoic acid	284	C18H36O2	000057-11-4	81



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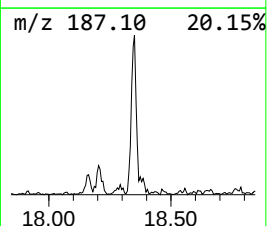
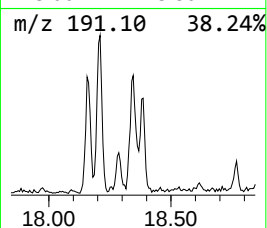
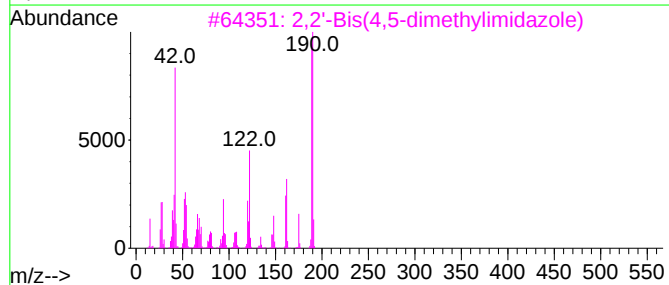
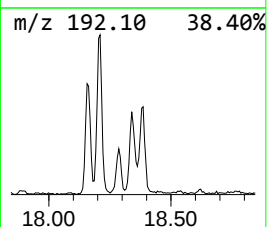
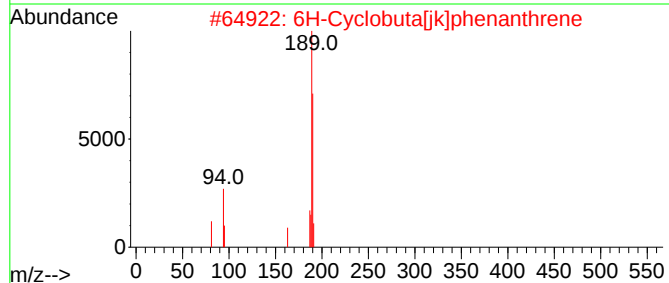
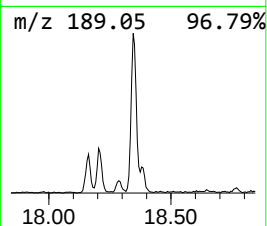
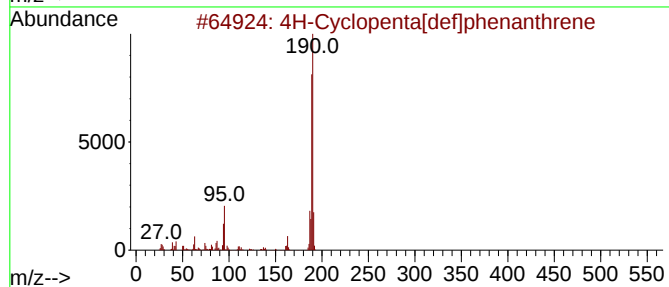
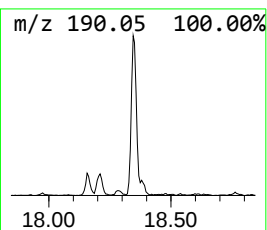
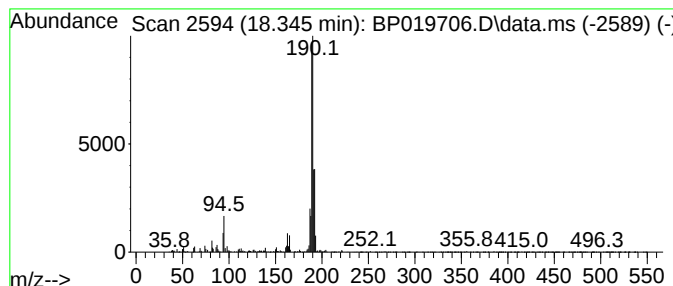
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.345	2.55 ng	136175	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	42
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
4			2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	35
5			4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021424\
Data File : BP019706.D
Acq On : 14 Feb 2024 17:47
Operator : MA/JU
Sample : P1449-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

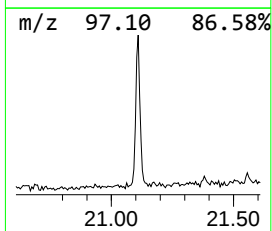
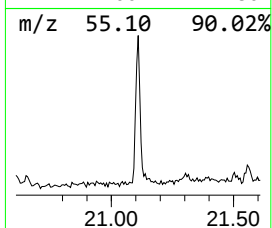
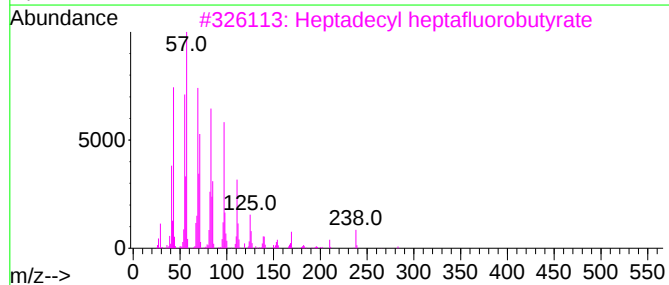
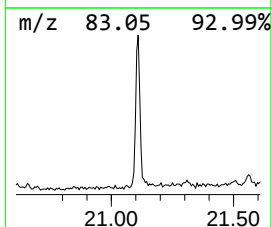
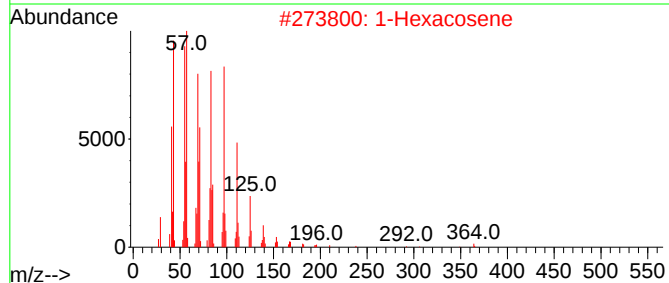
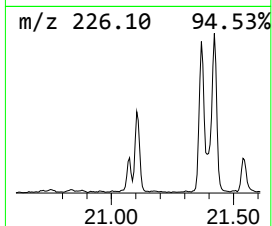
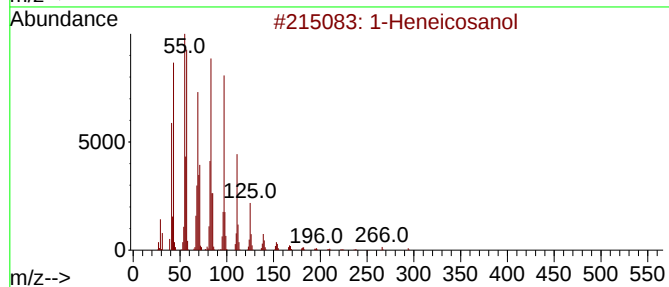
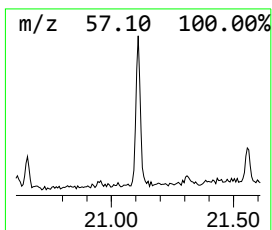
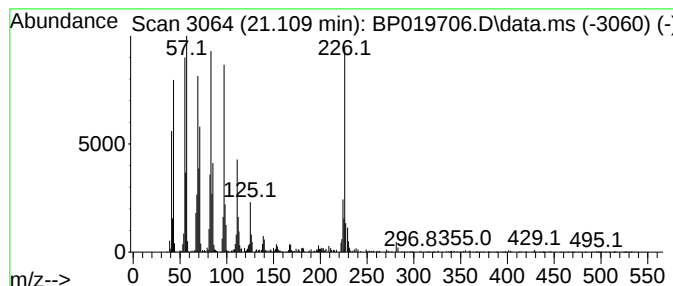
Instrument :
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ClientSampleId :
ETGI-362

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 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.110	4.30 ng	380221	Chrysene-d12	21.386	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	1-Hexacosene	364	C26H52	018835-33-1	91
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
5	Cyclohexadecane	224	C16H32	000295-65-8	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021424\
Data File : BP019706.D
Acq On : 14 Feb 2024 17:47
Operator : MA/JU
Sample : P1449-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
ETGI-362

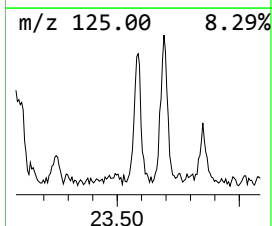
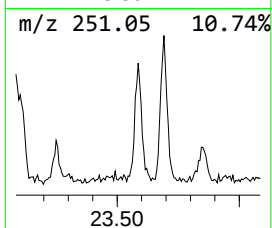
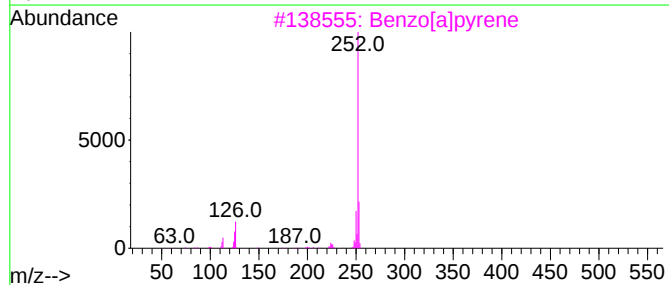
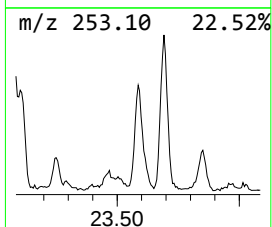
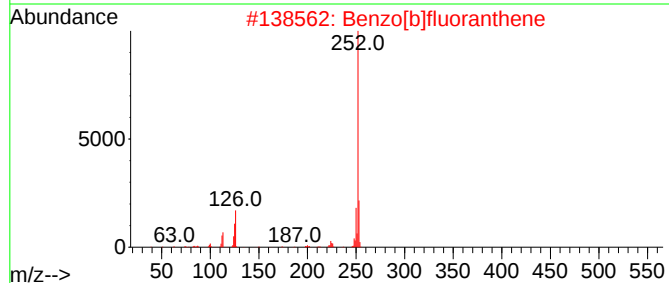
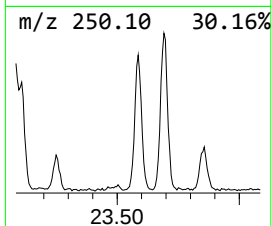
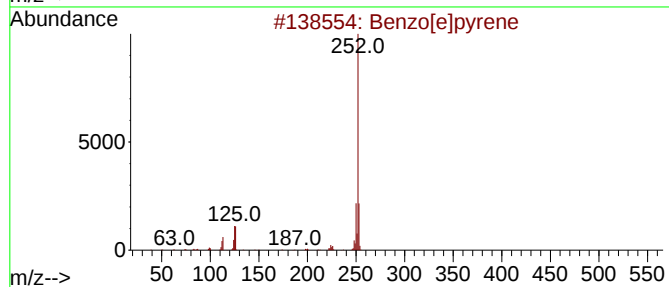
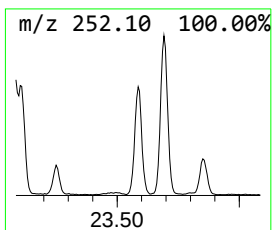
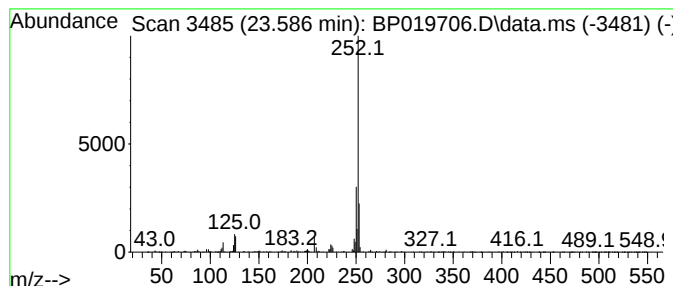
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.586	6.17 ng	346110	Perylene-d12	23.797

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	94
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3			Benzo[a]pyrene	252	C20H12	000050-32-8	90
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5			Perylene	252	C20H12	000198-55-0	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021424\
Data File : BP019706.D
Acq On : 14 Feb 2024 17:47
Operator : MA/JU
Sample : P1449-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
ETGI-362

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.628	5.0	ng	112249	1	7.904	446496	20.0
1-Phenoxypropan...	11.457	2.4	ng	71573	2	10.704	590675	20.0
unknown14.763	14.763	34.2	ng	1405820	3	14.533	823036	20.0
n-Hexadecanoic ...	18.192	8.3	ng	443422	4	17.292	1067560	20.0
4H-Cyclopenta[d...	18.345	2.5	ng	136175	4	17.292	1067560	20.0
1-Heneicosanol	21.110	4.3	ng	380221	5	21.386	1768390	20.0
Benzo[e]pyrene	23.586	6.2	ng	346110	6	23.797	1121700	20.0