

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
 Data File : BP005378.D
 Acq On : 22 Apr 2021 16:33
 Operator : CG/JU
 Sample : M2112-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 M-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-BP042121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005378.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.246	360	367	388	rBV	671711	958860	45.86%	6.742%
2	6.834	630	637	651	rBV	637943	1022409	48.89%	7.188%
3	7.640	766	774	783	rBV	153458	245570	11.74%	1.727%
4	8.804	963	972	984	rBV	399593	651347	31.15%	4.579%
5	10.434	1238	1249	1261	rBV	173416	305743	14.62%	2.150%
6	12.916	1664	1671	1683	rBV	869013	1287570	61.58%	9.053%
7	13.198	1712	1719	1728	rBV	173418	275389	13.17%	1.936%
8	13.769	1808	1816	1824	rBV	36793	59265	2.83%	0.417%
9	14.304	1897	1907	1914	rBV	273845	392364	18.76%	2.759%
10	15.439	2095	2100	2111	rBV2	39303	61151	2.92%	0.430%
11	15.810	2154	2163	2179	rBV	847383	1221548	58.42%	8.588%
12	16.975	2357	2361	2367	rBV3	15954	23108	1.11%	0.162%
13	17.069	2368	2377	2381	rBV	339289	500545	23.94%	3.519%
14	17.110	2381	2384	2389	rVB	66203	85875	4.11%	0.604%
15	17.969	2523	2530	2539	rBV2	119576	184514	8.82%	1.297%
16	18.133	2553	2558	2561	rBV3	16939	26438	1.26%	0.186%
17	18.257	2575	2579	2583	rBV5	13857	21135	1.01%	0.149%
18	18.480	2612	2617	2623	rVB2	24581	36051	1.72%	0.253%
19	19.092	2714	2721	2728	rBV	348436	490509	23.46%	3.449%
20	19.210	2738	2741	2744	rBV3	34123	38849	1.86%	0.273%
21	19.445	2771	2781	2789	rBV	284267	441109	21.10%	3.101%
22	19.645	2809	2815	2820	rBV	1769473	2091030	100.00%	14.702%
23	19.927	2859	2863	2870	rVB2	45766	81571	3.90%	0.574%
24	20.027	2877	2880	2884	rBV2	26438	31471	1.51%	0.221%
25	20.080	2887	2889	2893	rVB2	17970	21669	1.04%	0.152%
26	20.663	2985	2988	2995	rVB	33126	46438	2.22%	0.326%
27	20.821	3012	3015	3019	rBV2	34678	51079	2.44%	0.359%
28	20.886	3023	3026	3033	rVV3	159969	245632	11.75%	1.727%
29	20.957	3035	3038	3043	rVB	37199	46652	2.23%	0.328%
30	21.168	3068	3074	3078	rBV2	573149	922282	44.11%	6.484%
31	21.204	3078	3080	3090	rVB	228608	277042	13.25%	1.948%
32	21.321	3097	3100	3105	rVB2	36599	45333	2.17%	0.319%
33	21.710	3163	3166	3170	rBV3	53391	73625	3.52%	0.518%
34	21.768	3174	3176	3184	rVB5	58547	107822	5.16%	0.758%
35	22.010	3213	3217	3221	rBV2	90596	122073	5.84%	0.858%
36	22.445	3288	3291	3295	rBV2	52179	58062	2.78%	0.408%

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005378.D
Acq On : 22 Apr 2021 16:33
Operator : CG/JU
Sample : M2112-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
M-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-BP042121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.745	3336	3342	3346	rBV	246079	559490	26.76%	3.934%
38	23.233	3420	3425	3432	rVB	141711	252699	12.08%	1.777%
39	23.327	3437	3441	3449	rVB	169550	306884	14.68%	2.158%
40	23.427	3453	3458	3464	rBV	316802	552905	26.44%	3.887%

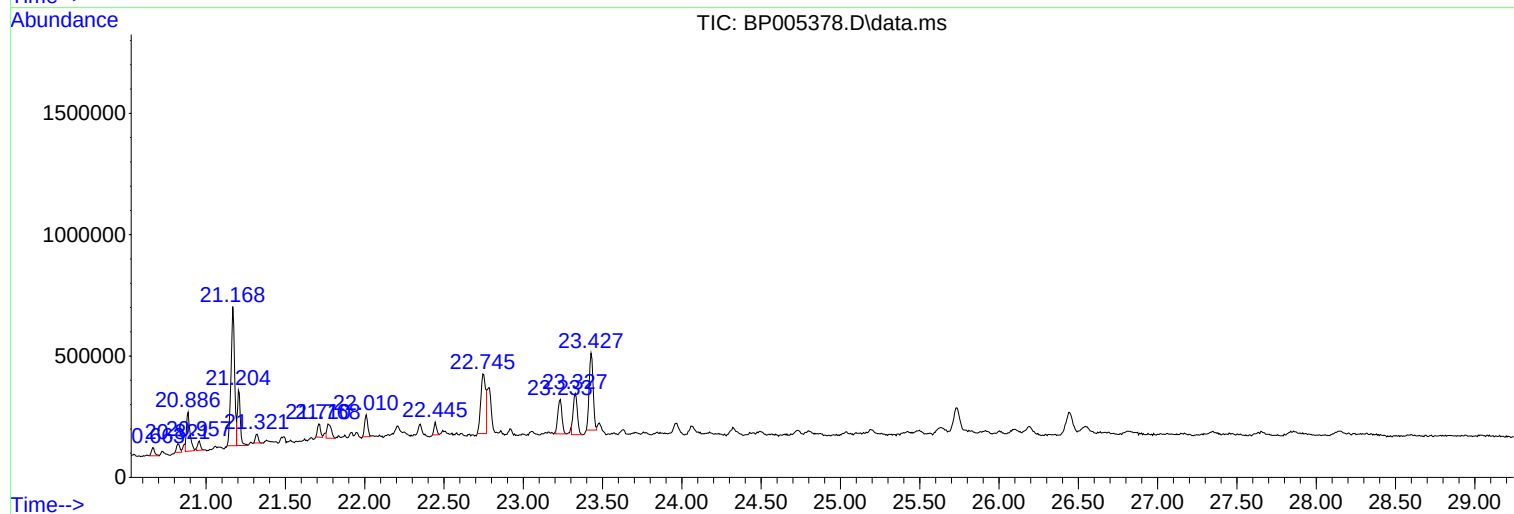
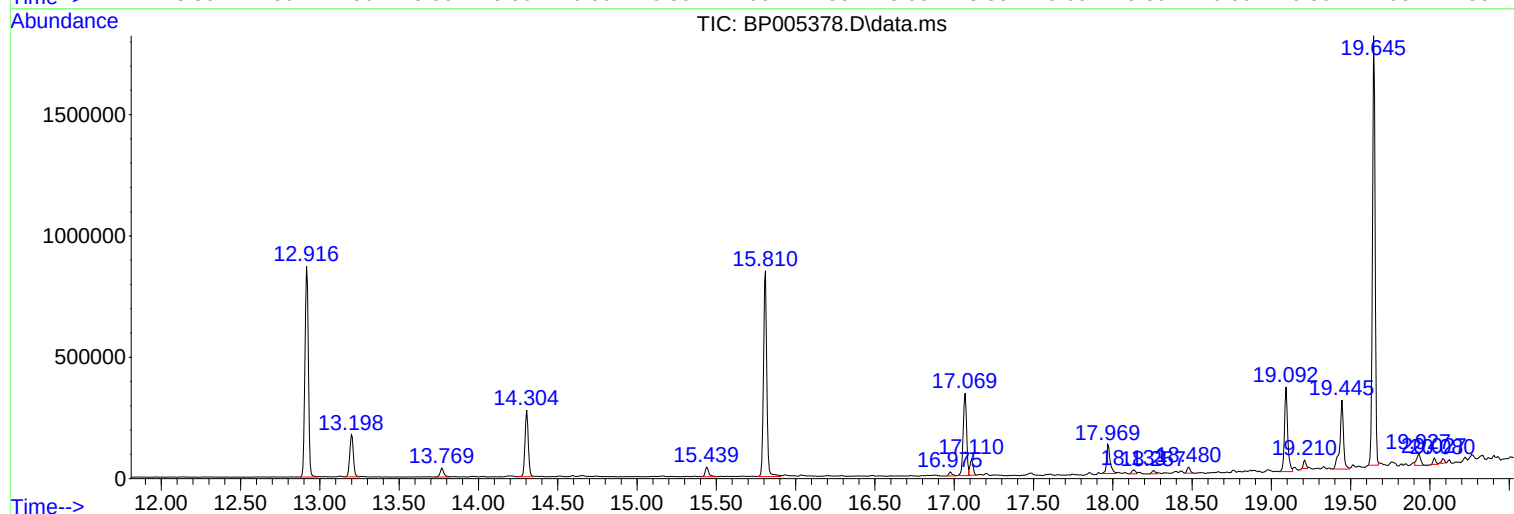
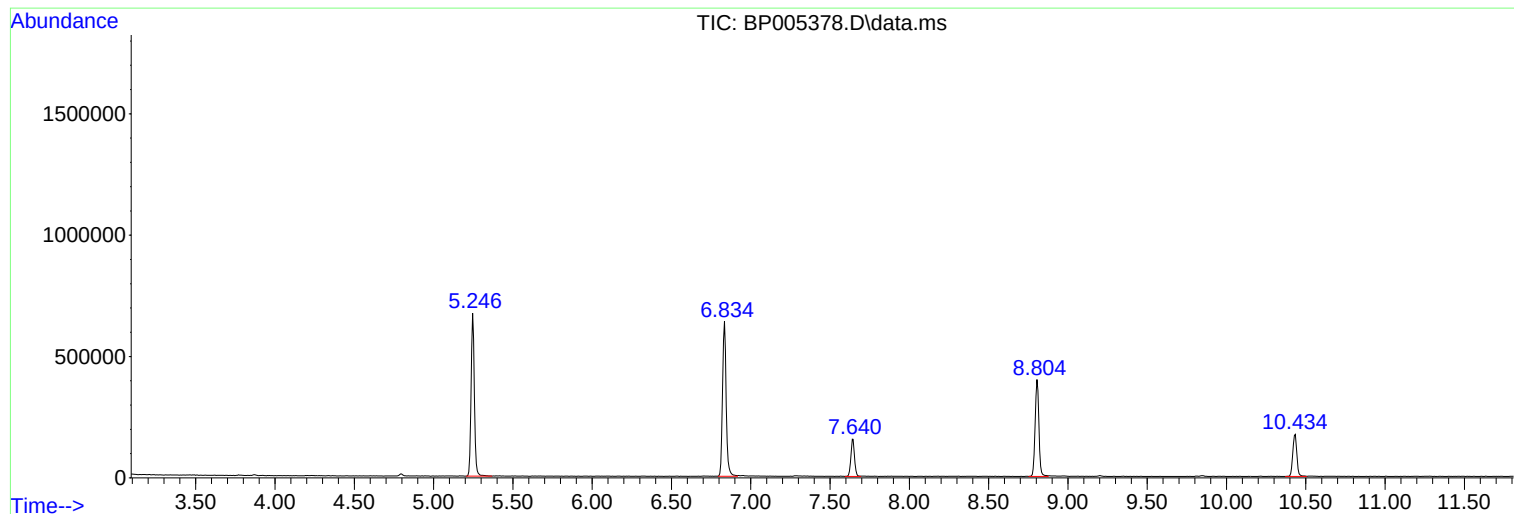
Sum of corrected areas: 14223108

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005378.D
Acq On : 22 Apr 2021 16:33
Operator : CG/JU
Sample : M2112-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampled :
M-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005378.D
Acq On : 22 Apr 2021 16:33
Operator : CG/JU
Sample : M2112-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

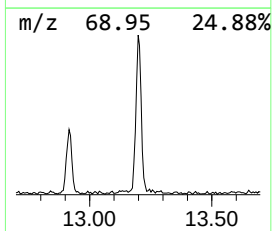
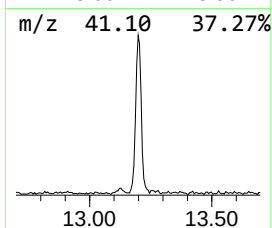
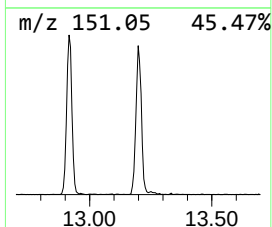
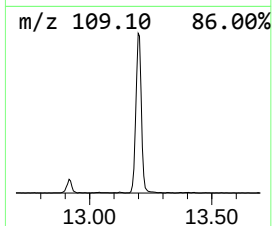
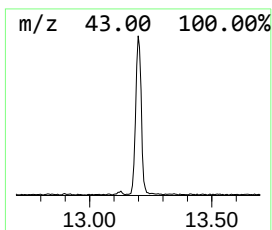
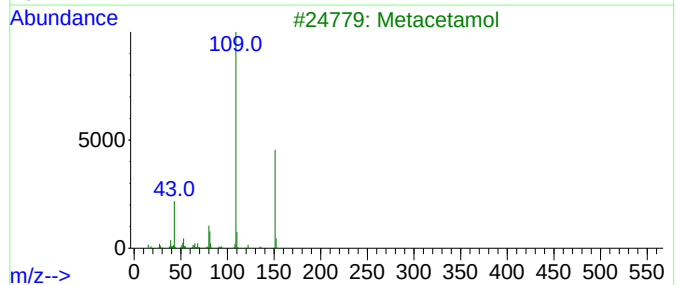
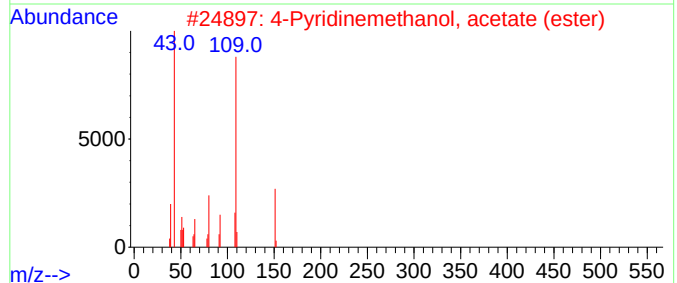
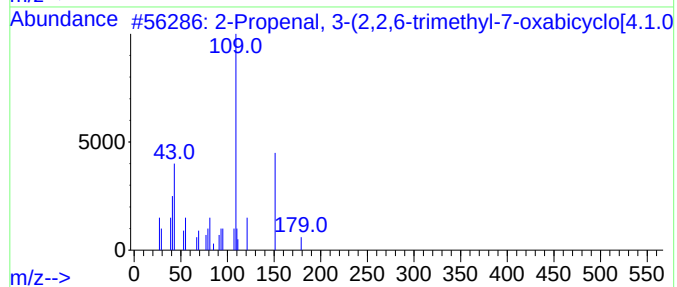
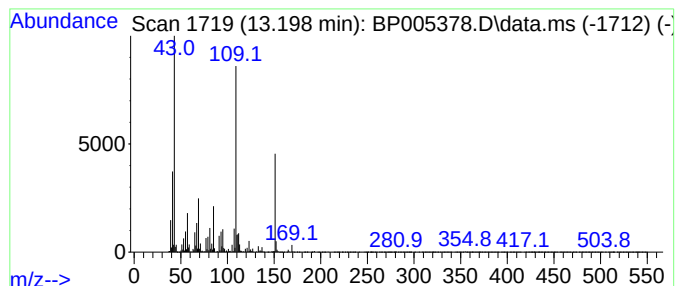
Instrument :
BNA_P
ClientSampleId :
M-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.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-Propenal, 3-(2,2,6-trimet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.198	14.04 ng	275389	Acenaphthene-d10		14.304	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Propenal, 3-(2,2,6-trimethyl-7...		194	C12H18O2	055759-91-6	64
2	4-Pyridinemethanol, acetate (ester)		151	C8H9NO2	001007-48-3	52
3	Metacetamol		151	C8H9NO2	000621-42-1	52
4	Pyridine, 3-butyl-, 1-oxide		151	C9H13NO	031396-33-5	52
5	Acetaminophen		151	C8H9NO2	000103-90-2	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005378.D
Acq On : 22 Apr 2021 16:33
Operator : CG/JU
Sample : M2112-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
M-1

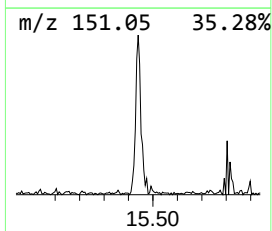
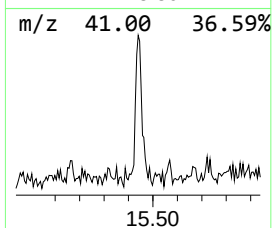
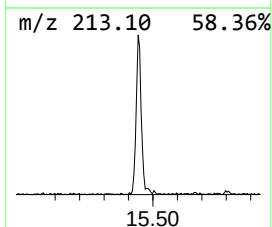
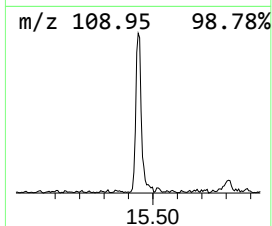
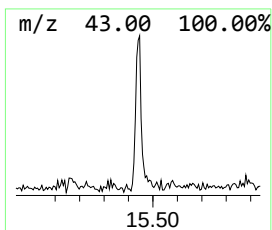
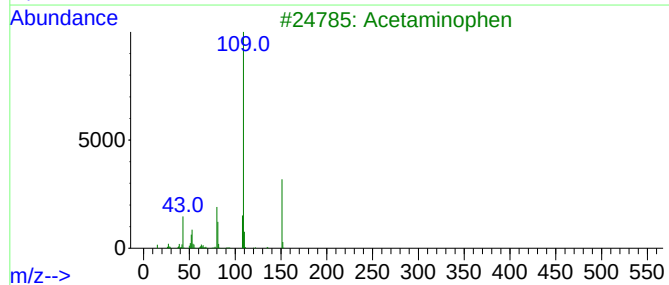
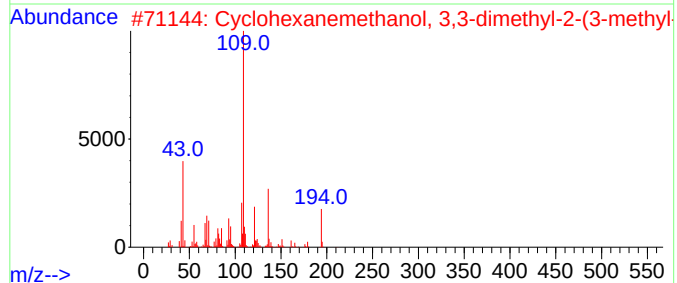
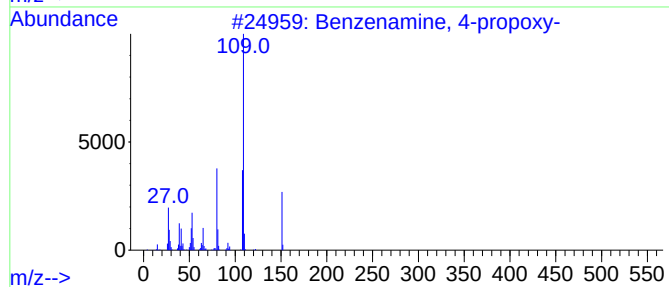
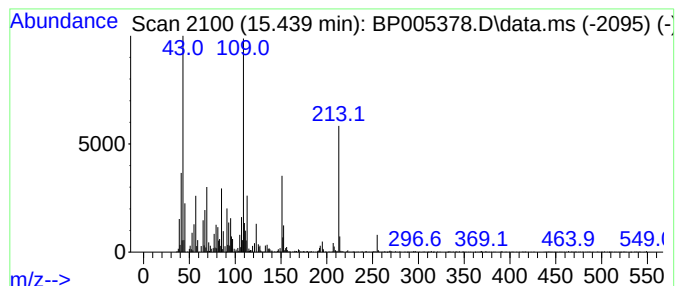
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown15.43 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.439	3.12 ng	61151	Acenaphthene-d10	14.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenamine, 4-propoxy-	151	C9H13NO	004469-80-1	38
2			Cyclohexanemethanol, 3,3-dimethy...	212	C13H24O2	072541-28-7	38
3			Acetaminophen	151	C8H9NO2	000103-90-2	35
4			Metacetamol	151	C8H9NO2	000621-42-1	35
5			2-Cyclohexen-1-ol, 2-methyl-5-(1...	152	C10H16O	001197-06-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005378.D
Acq On : 22 Apr 2021 16:33
Operator : CG/JU
Sample : M2112-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
M-1

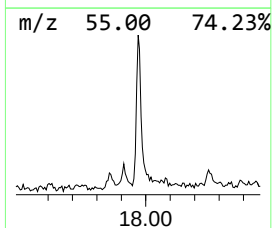
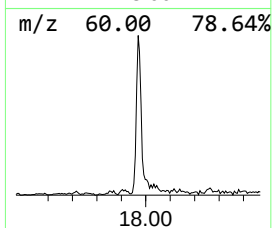
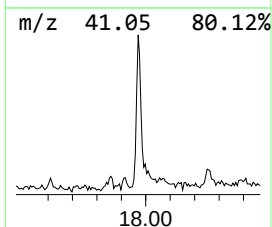
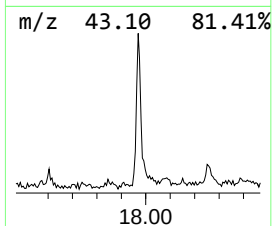
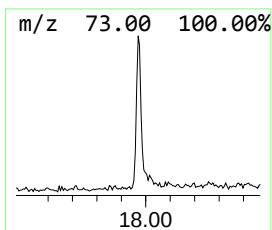
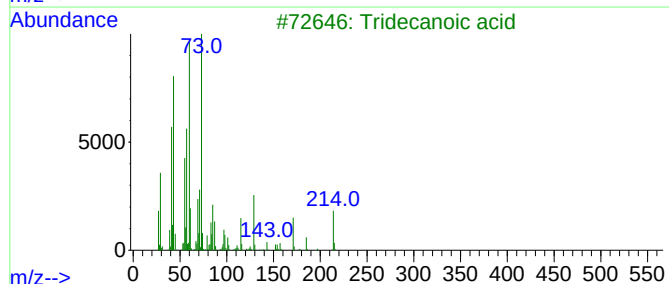
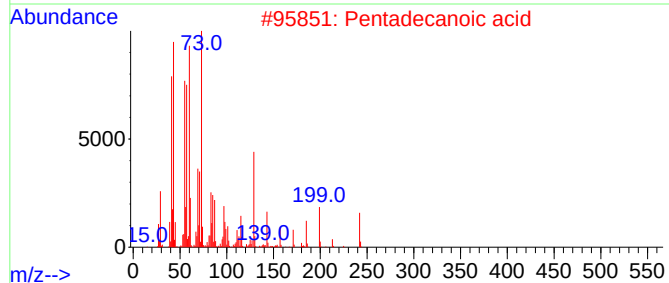
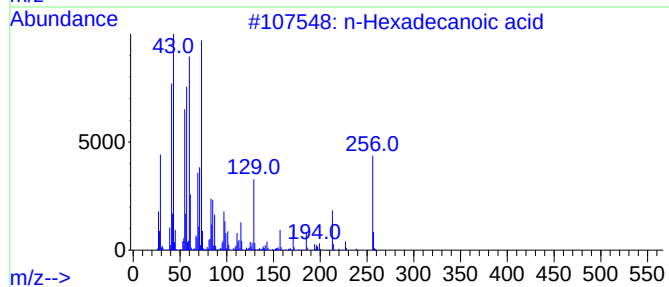
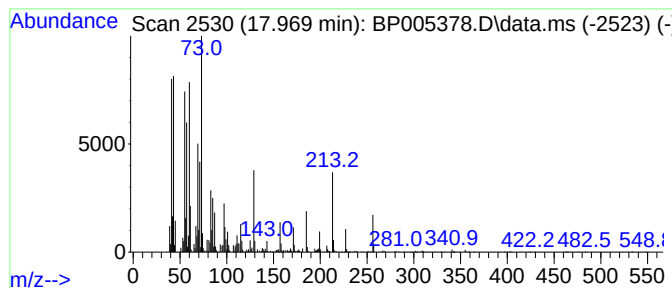
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.969	7.37 ng	184514	Phenanthrene-d10	17.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			Octadecanoic acid	284	C18H36O2	000057-11-4	62
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005378.D
Acq On : 22 Apr 2021 16:33
Operator : CG/JU
Sample : M2112-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
M-1

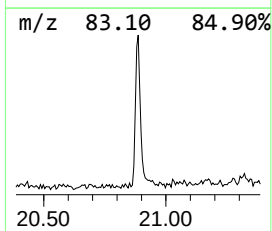
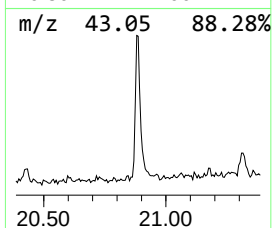
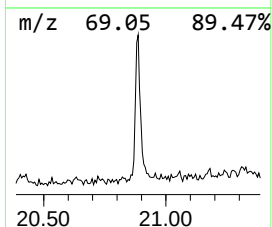
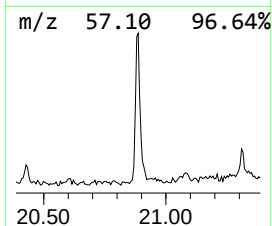
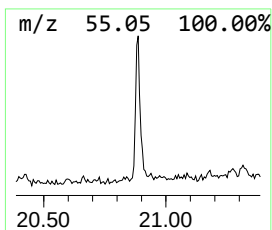
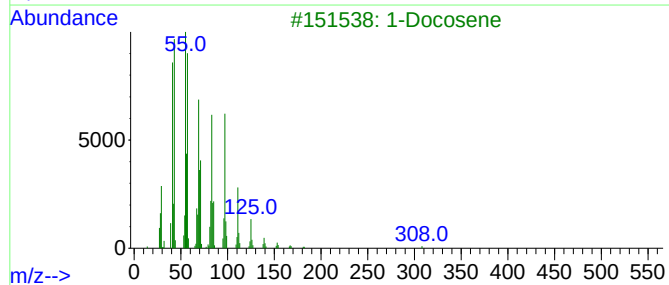
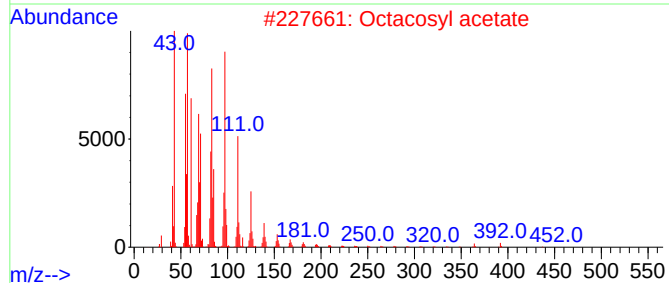
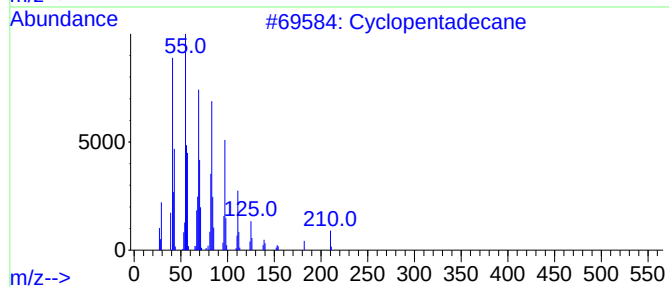
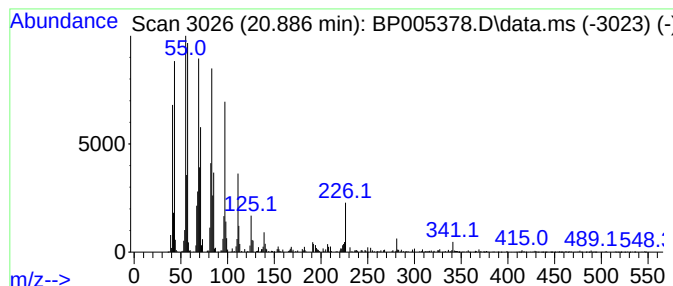
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.886	5.33 ng	245632	Chrysene-d12	21.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	98
2			Octacosyl acetate	452	C30H60O2	018206-97-8	95
3			1-Docosene	308	C22H44	001599-67-3	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			Cyclohexadecane	224	C16H32	000295-65-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005378.D
Acq On : 22 Apr 2021 16:33
Operator : CG/JU
Sample : M2112-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampled :
M-1

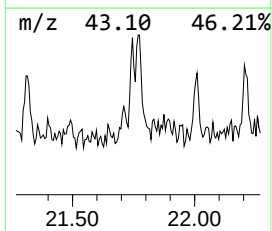
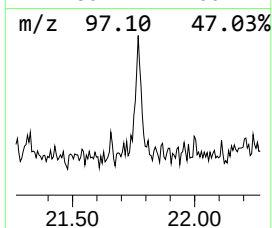
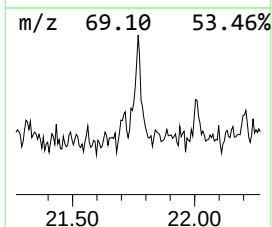
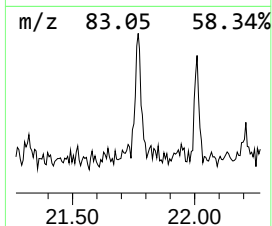
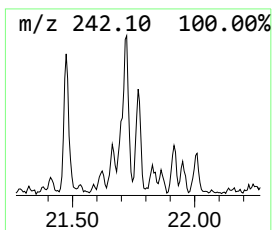
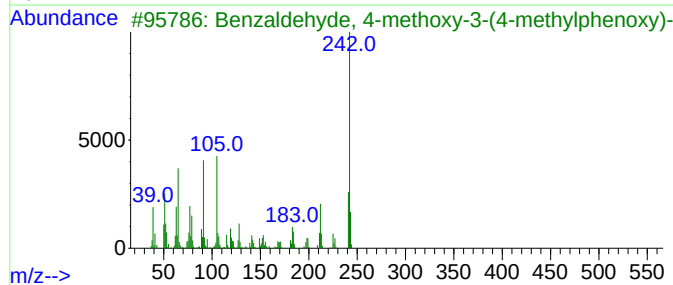
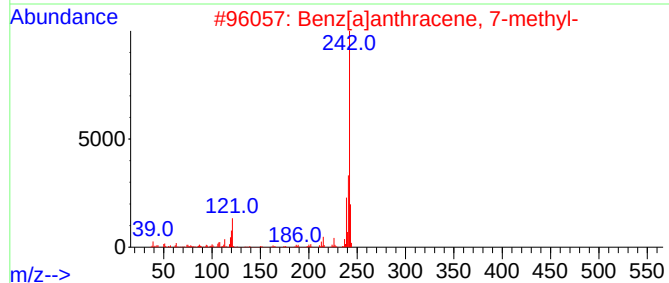
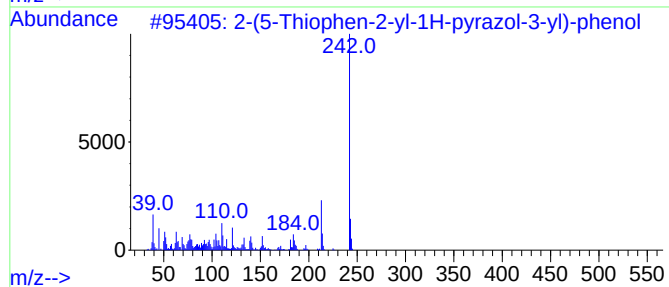
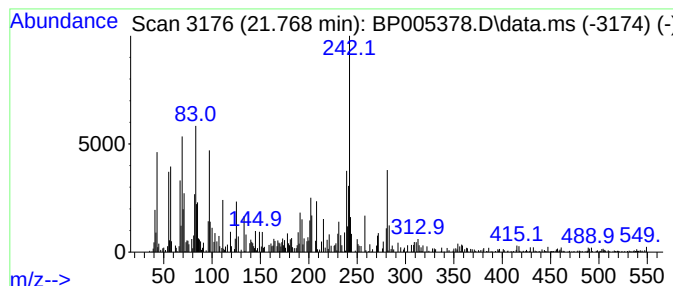
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown21.76 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.768	2.34 ng	107822	Chrysene-d12	21.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(5-Thiophen-2-yl-1H-pyrazol-3-...	242	C13H10N2OS	1000301-11-6	46		
2	Benz[a]anthracene, 7-methyl-	242	C19H14	002541-69-7	41		
3	Benzaldehyde, 4-methoxy-3-(4-met...	242	C15H14O3	093899-03-7	38		
4	2-Methylchrysene	242	C19H14	003351-32-4	38		
5	Fenopropfen	242	C15H14O3	031879-05-7	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005378.D
Acq On : 22 Apr 2021 16:33
Operator : CG/JU
Sample : M2112-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
M-1

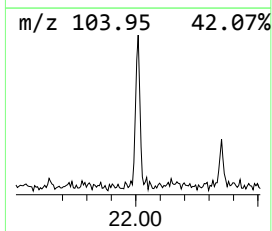
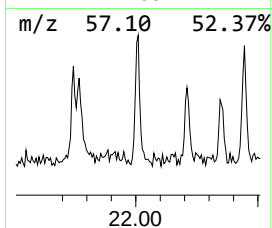
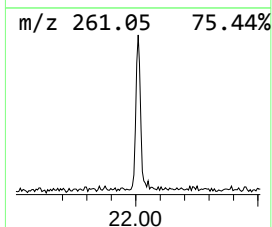
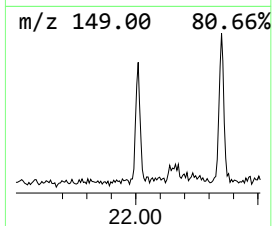
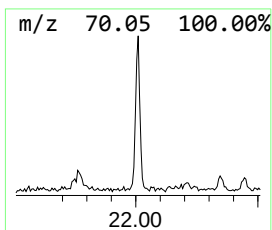
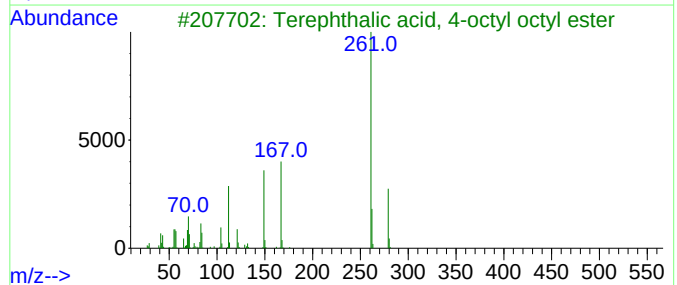
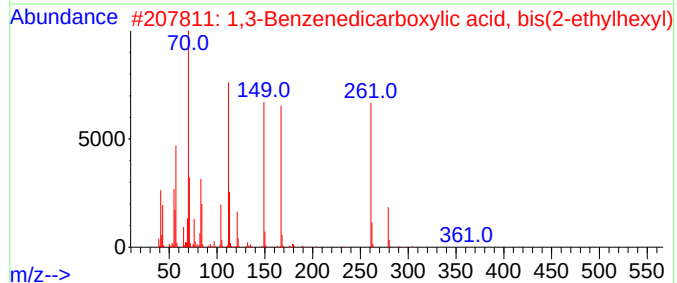
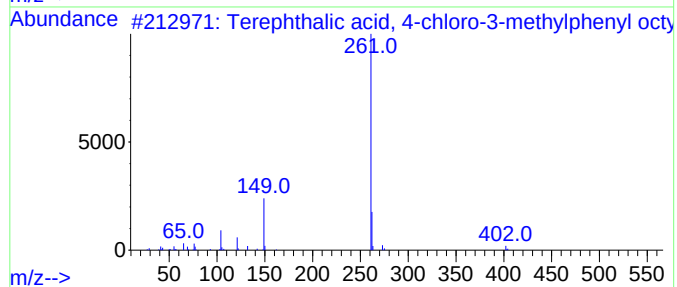
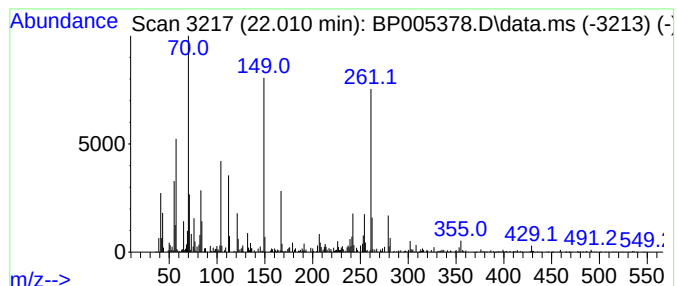
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Terephthalic acid, 4-chloro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.010	2.65 ng	122073	Chrysene-d12	21.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Terephthalic acid, 4-chloro-3-me...	402	C23H27ClO4	1000323-70-4	53
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38
3			Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	35
4			Isophthalic acid, 4-methoxypheny...	384	C23H28O5	1000344-48-2	27
5			Isophthalic acid, octyl 1-propyl...	376	C23H36O4	1000356-40-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005378.D
Acq On : 22 Apr 2021 16:33
Operator : CG/JU
Sample : M2112-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
M-1

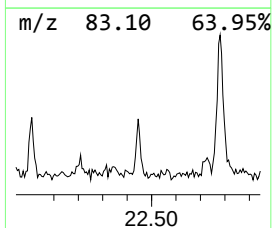
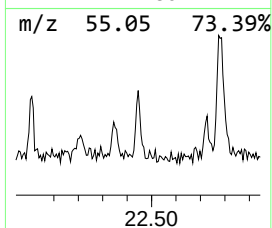
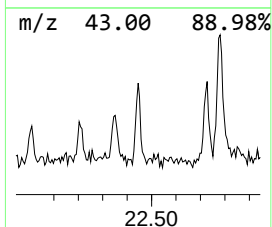
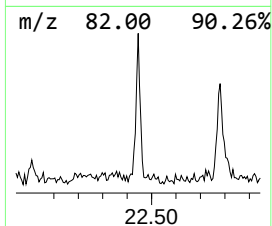
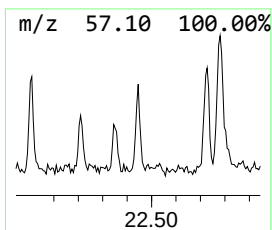
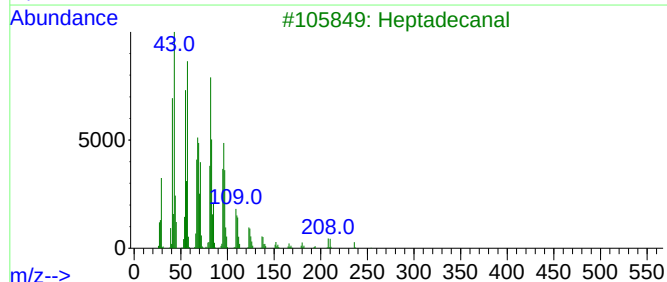
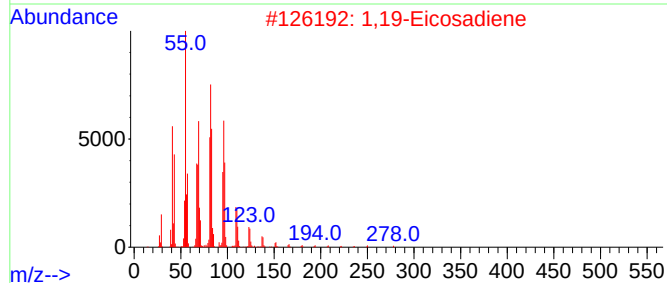
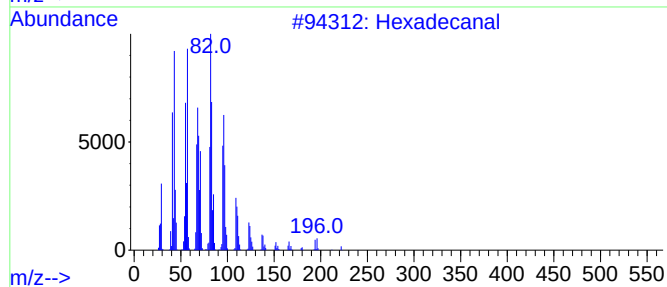
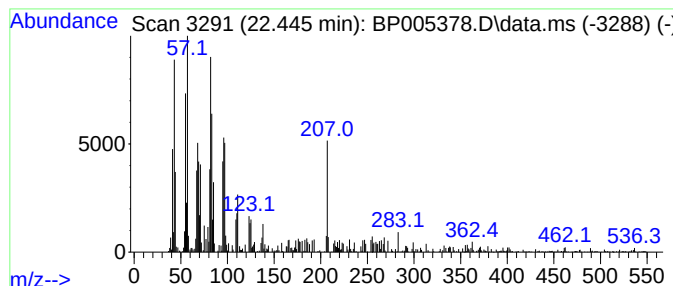
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.445	2.10 ng	58062	Perylene-d12	23.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanal	240	C16H32O	000629-80-1	70
2			1,19-Eicosadiene	278	C20H38	014811-95-1	68
3			Heptadecanal	254	C17H34O	1000376-70-0	62
4			trans-2-Dodecen-1-ol	184	C12H24O	069064-37-5	60
5			Tetradecanal	212	C14H28O	000124-25-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005378.D
Acq On : 22 Apr 2021 16:33
Operator : CG/JU
Sample : M2112-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
M-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.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-Propenal, 3-(...	13.198	14.0	ng	275389	3	14.304	392364	20.0
unknown15.43	15.439	3.1	ng	61151	3	14.304	392364	20.0
n-Hexadecanoic ...	17.969	7.4	ng	184514	4	17.069	500545	20.0
Cyclopentadecane	20.886	5.3	ng	245632	5	21.169	922282	20.0
unknown21.76	21.768	2.3	ng	107822	5	21.169	922282	20.0
Terephthalic ac...	22.010	2.6	ng	122073	5	21.169	922282	20.0
Hexadecanal	22.445	2.1	ng	58062	6	23.427	552905	20.0