

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
 Data File : BM042544.D
 Acq On : 01 Nov 2023 17:48
 Operator : MA/JU
 Sample : 05164-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 ETGI-352

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_M\Methods\8270-BM103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042544.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	304	309	316	rBV	48880	69272	1.85%	0.265%
2	5.457	379	386	397	rBV	1179739	1684554	45.05%	6.450%
3	7.087	656	663	682	rBV	1188051	1847530	49.41%	7.074%
4	7.922	798	805	818	rVB	353692	558897	14.95%	2.140%
5	9.122	1000	1009	1016	rBV	702730	1162638	31.09%	4.452%
6	10.739	1272	1284	1301	rBV	446090	756690	20.24%	2.897%
7	13.192	1694	1701	1713	rBV	1730300	2401161	64.22%	9.194%
8	13.416	1733	1739	1751	rBV	139751	216555	5.79%	0.829%
9	14.569	1929	1935	1943	rBV	676872	953771	25.51%	3.652%
10	16.063	2182	2189	2200	rBV	1487318	2061688	55.14%	7.894%
11	17.321	2393	2403	2407	rBV	841092	1157839	30.97%	4.433%
12	17.362	2407	2410	2416	rVV	170056	240807	6.44%	0.922%
13	17.457	2419	2426	2433	rVB	34515	61884	1.66%	0.237%
14	17.745	2468	2475	2480	rBV	20192	37955	1.02%	0.145%
15	18.174	2542	2548	2556	rBV	664542	931736	24.92%	3.568%
16	18.392	2580	2585	2589	rBV3	36903	65374	1.75%	0.250%
17	18.756	2643	2647	2653	rVB3	32504	49497	1.32%	0.190%
18	19.309	2738	2741	2743	rBV2	43865	53200	1.42%	0.204%
19	19.374	2747	2752	2760	rVB	573268	812577	21.73%	3.111%
20	19.451	2760	2765	2772	rBV	331721	481473	12.88%	1.844%
21	19.656	2796	2800	2804	rVB3	63783	86658	2.32%	0.332%
22	19.703	2804	2808	2811	rBV3	102612	153336	4.10%	0.587%
23	19.745	2811	2815	2822	rVB	479790	612946	16.39%	2.347%
24	19.939	2842	2848	2855	rBV	3053761	3739066	100.00%	14.317%
25	20.186	2887	2890	2895	rBV3	56080	94280	2.52%	0.361%
26	20.333	2912	2915	2918	rBV	46147	57403	1.54%	0.220%
27	20.533	2946	2949	2953	rBV2	40685	57923	1.55%	0.222%
28	20.686	2972	2975	2977	rBV2	59436	58676	1.57%	0.225%
29	21.168	3051	3057	3064	rVB3	323949	637816	17.06%	2.442%
30	21.368	3088	3091	3097	rBV	259935	294714	7.88%	1.128%
31	21.503	3108	3114	3118	rBV2	1029929	1593119	42.61%	6.100%
32	21.545	3118	3121	3125	rVB	310440	367737	9.83%	1.408%
33	22.339	3253	3256	3263	rVB	179476	218097	5.83%	0.835%
34	23.174	3392	3398	3404	rBV2	418153	1012191	27.07%	3.876%
35	23.703	3485	3488	3498	rVB	226444	404083	10.81%	1.547%
36	23.927	3520	3526	3531	rBV	593066	1122546	30.02%	4.298%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042544.D
Acq On : 01 Nov 2023 17:48
Operator : MA/JU
Sample : 05164-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI-352

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_M\Methods\8270-BM103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

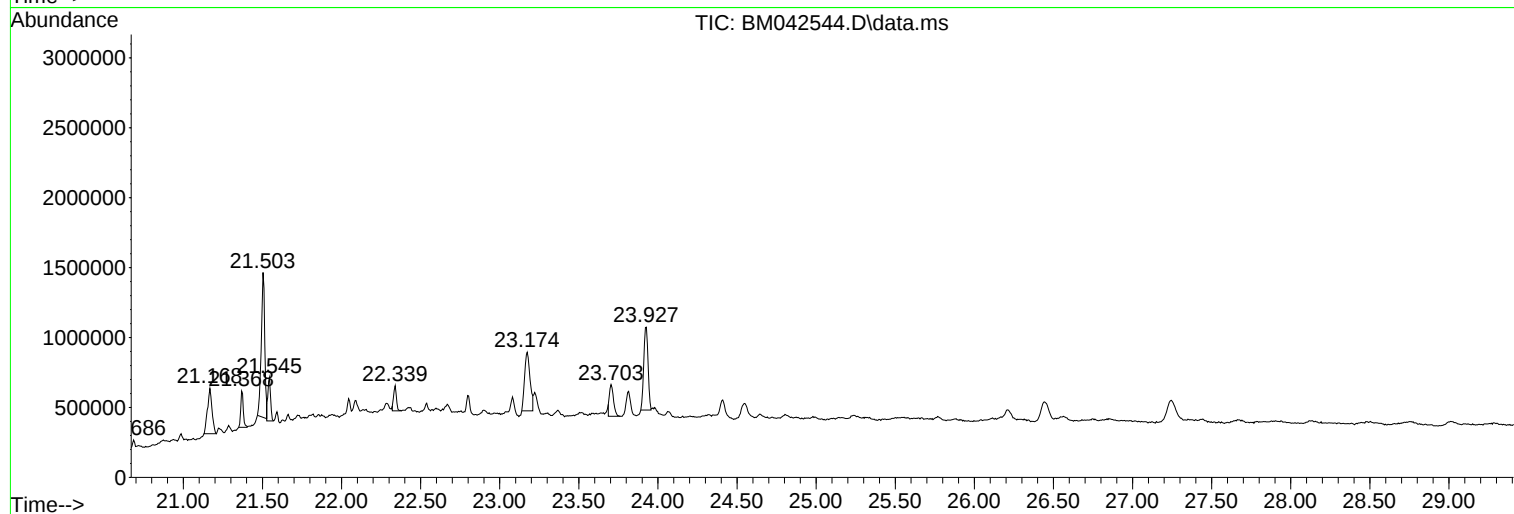
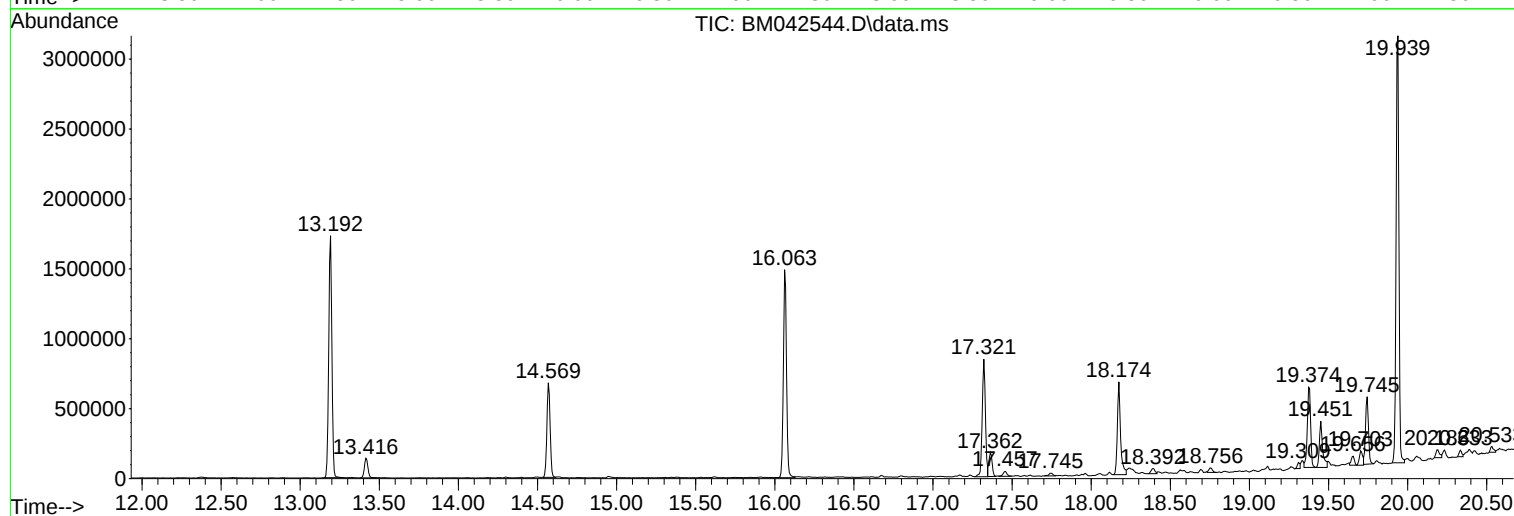
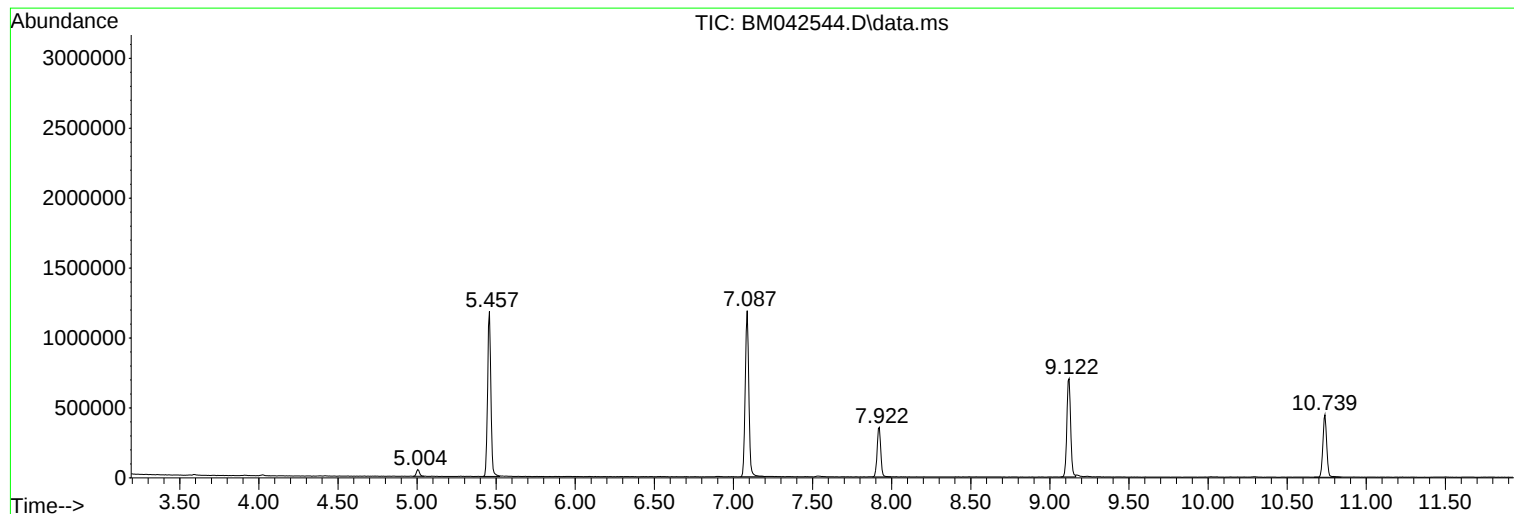
Sum of corrected areas: 26115689

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042544.D
Acq On : 01 Nov 2023 17:48
Operator : MA/JU
Sample : 05164-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI-352

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042544.D
Acq On : 01 Nov 2023 17:48
Operator : MA/JU
Sample : 05164-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI-352

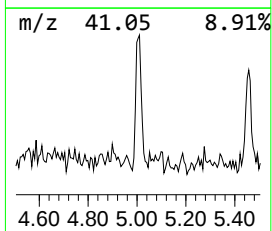
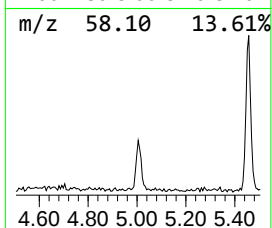
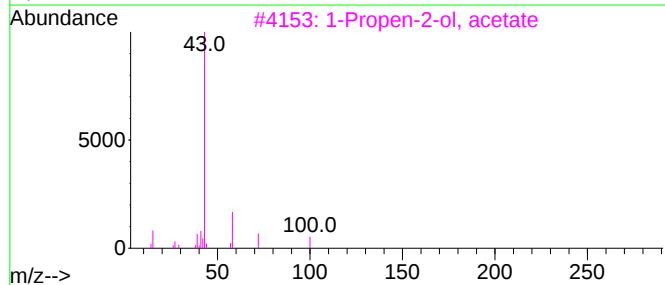
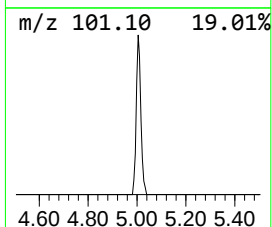
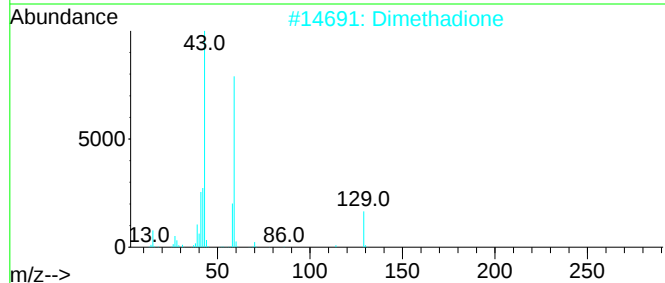
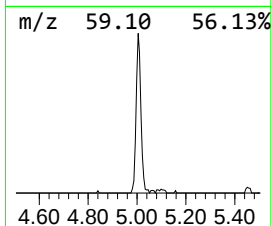
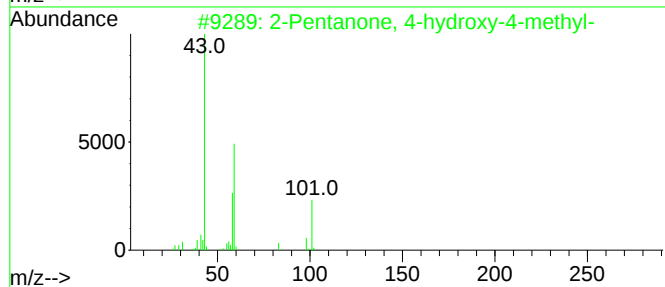
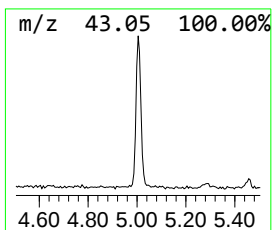
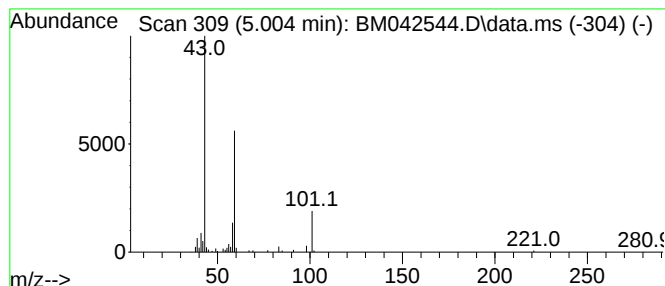
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.48 ng	69272	1,4-Dichlorobenzene-d4	7.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Dimethadione	129	C5H7NO3	000695-53-4	42
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5		Diacetamide	101	C4H7NO2	000625-77-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042544.D
Acq On : 01 Nov 2023 17:48
Operator : MA/JU
Sample : 05164-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI-352

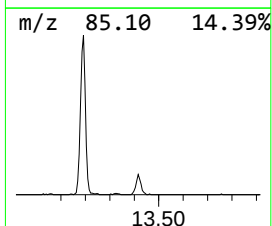
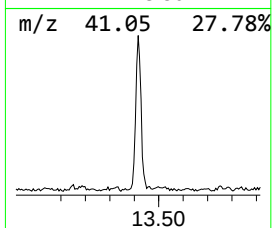
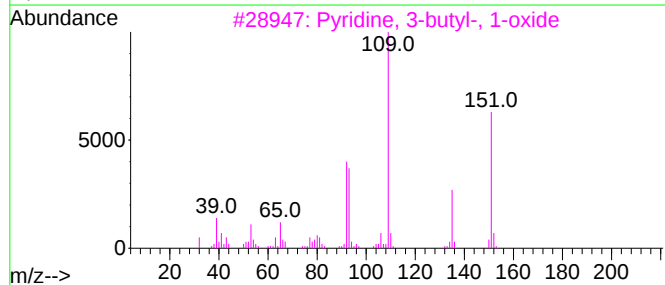
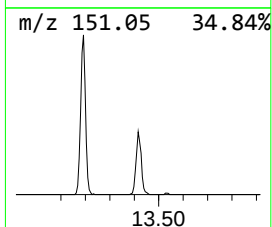
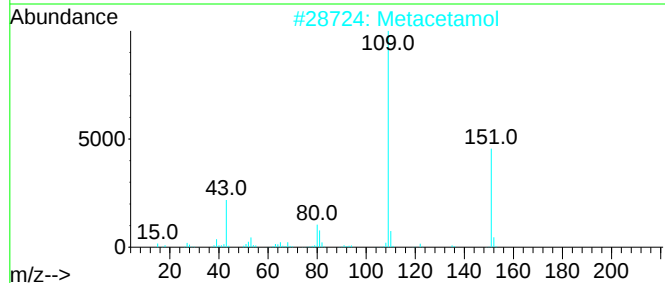
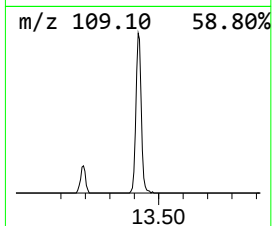
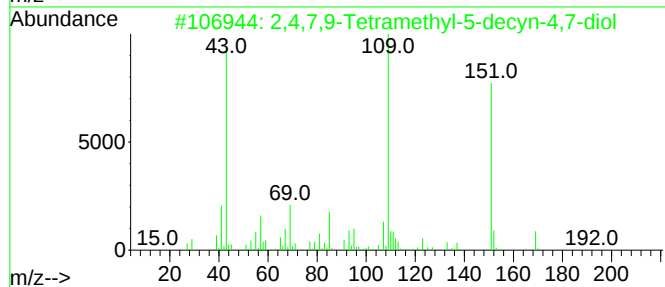
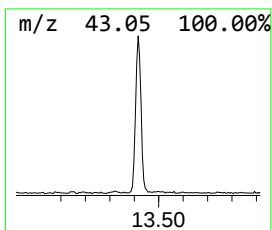
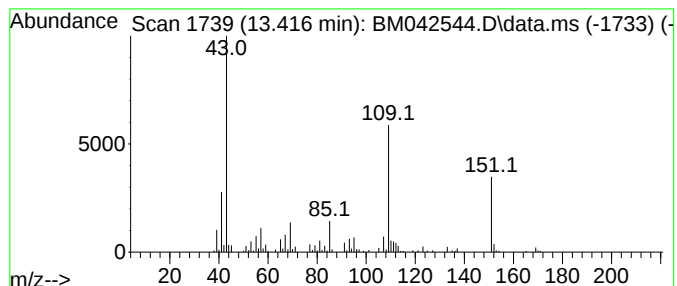
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.416	4.54 ng	216555	Acenaphthene-d10	14.569

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87	
2	Metacetamol	151	C8H9NO2	000621-42-1	49	
3	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	47	
4	Acetaminophen	151	C8H9NO2	000103-90-2	47	
5	4-Amino-2-methylpyrimidine	109	C5H7N3	000074-69-1	43	



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042544.D
Acq On : 01 Nov 2023 17:48
Operator : MA/JU
Sample : 05164-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI-352

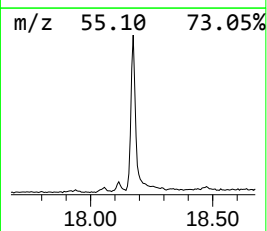
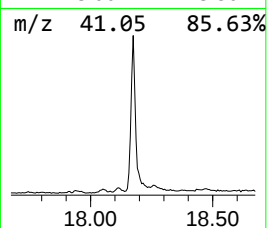
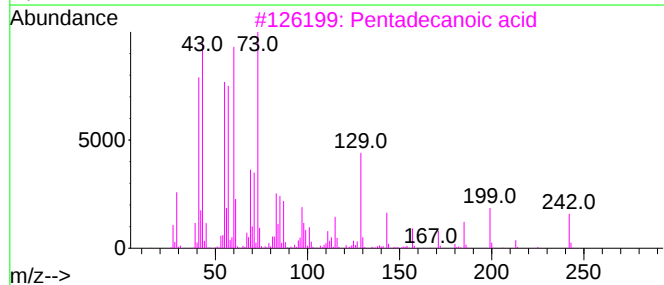
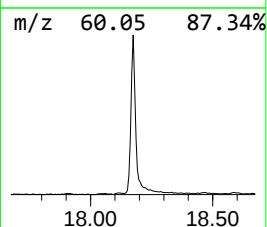
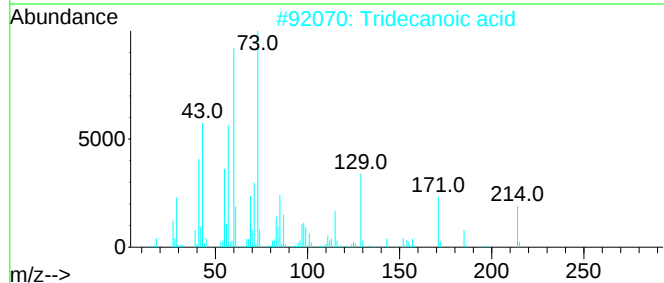
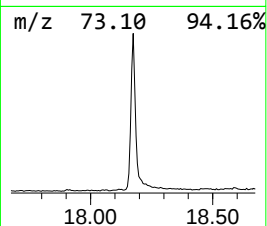
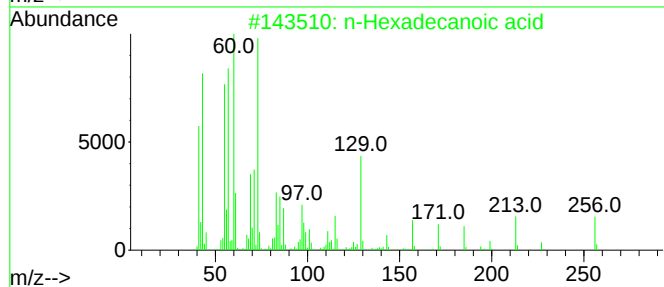
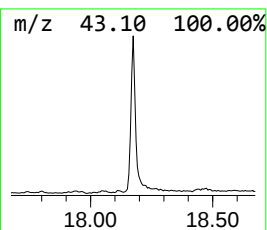
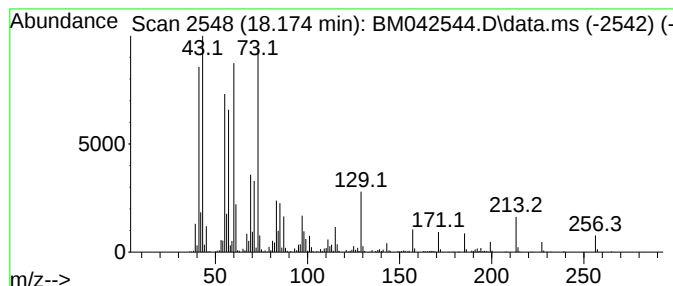
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	16.09 ng	931736	Phenanthrene-d10	17.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042544.D
Acq On : 01 Nov 2023 17:48
Operator : MA/JU
Sample : 05164-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI-352

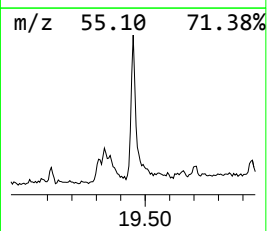
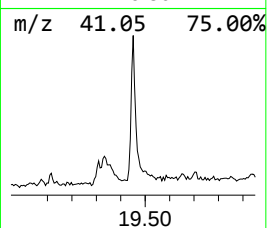
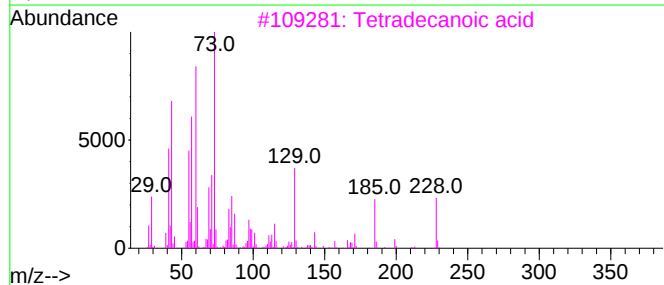
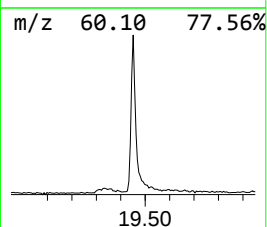
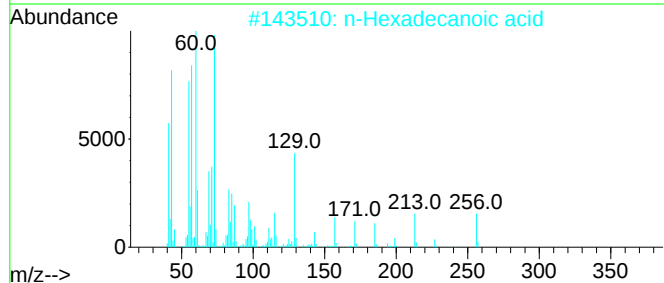
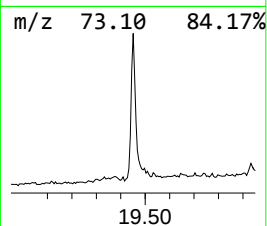
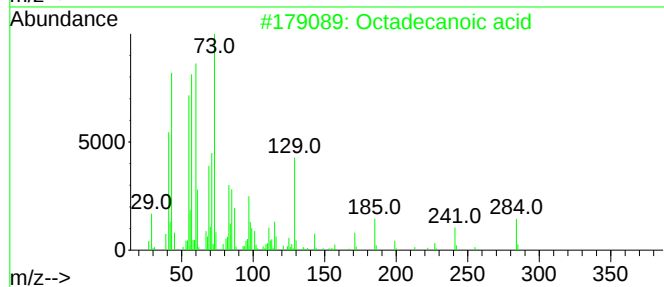
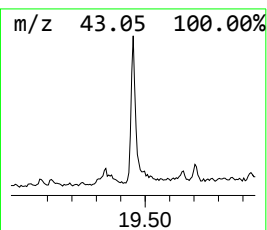
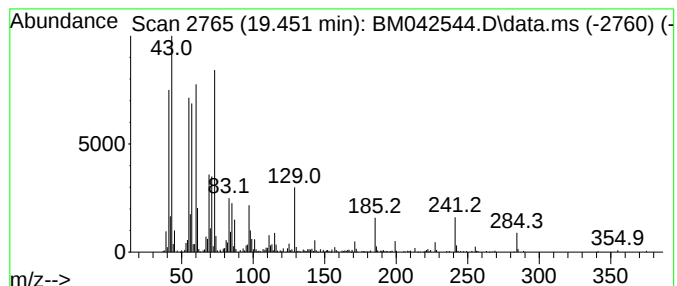
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	6.04 ng	481473	Chrysene-d12	21.503

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			Heptanoic acid	130	C7H14O2	000111-14-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042544.D
Acq On : 01 Nov 2023 17:48
Operator : MA/JU
Sample : 05164-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI-352

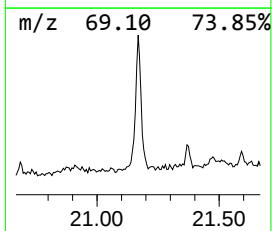
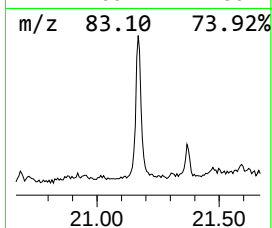
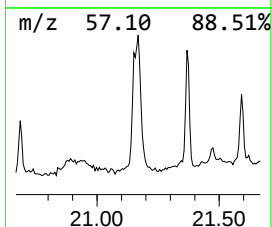
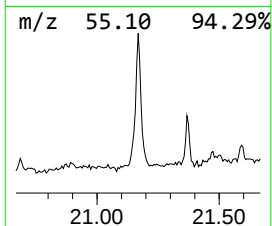
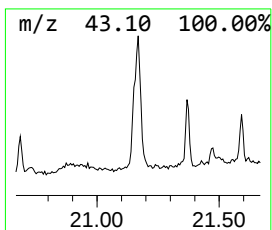
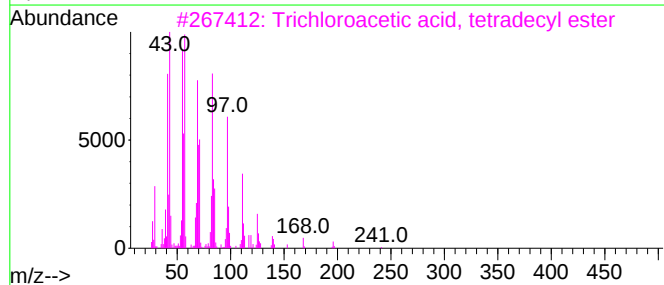
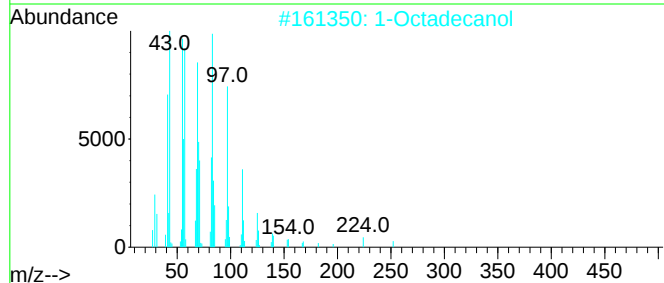
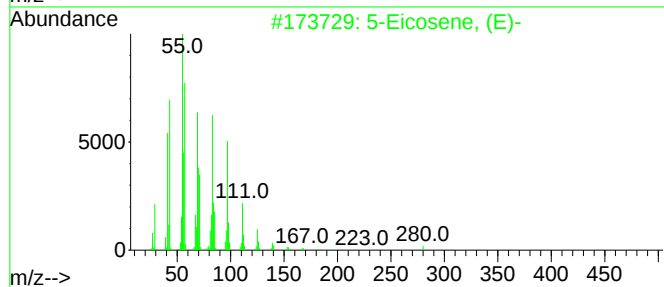
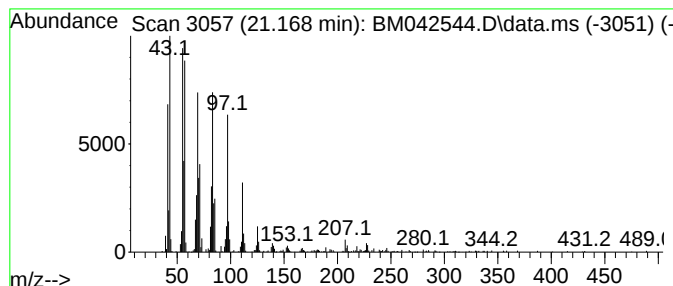
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.168	8.01 ng	637816	Chrysene-d12	21.503

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2			1-Octadecanol	270	C18H38O	000112-92-5	94
3			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	94
4			1-Hexacosene	364	C26H52	018835-33-1	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042544.D
Acq On : 01 Nov 2023 17:48
Operator : MA/JU
Sample : 05164-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI-352

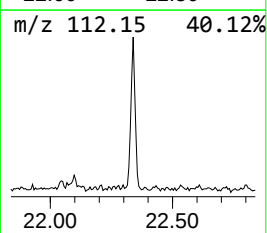
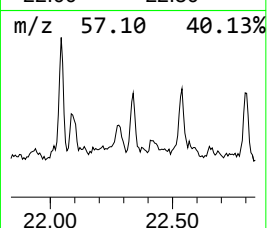
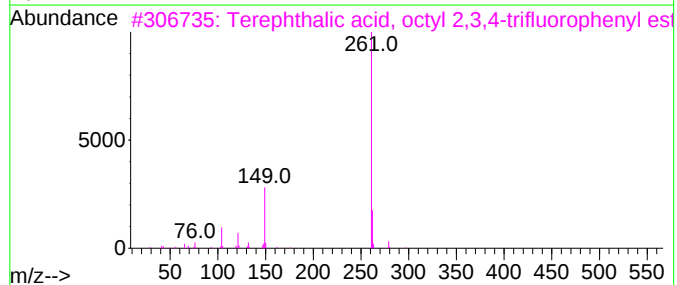
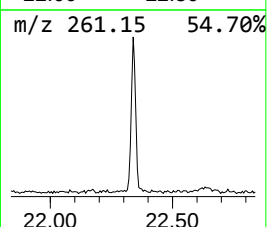
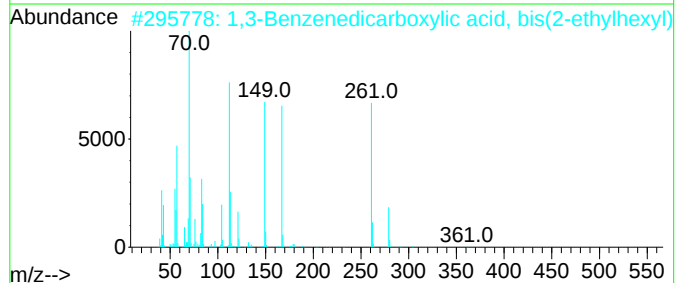
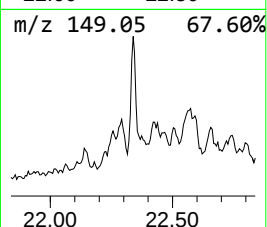
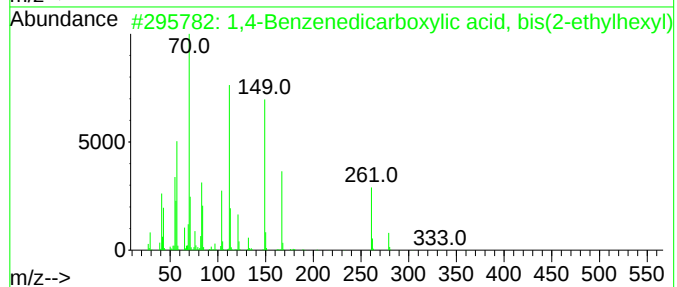
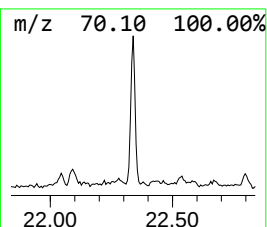
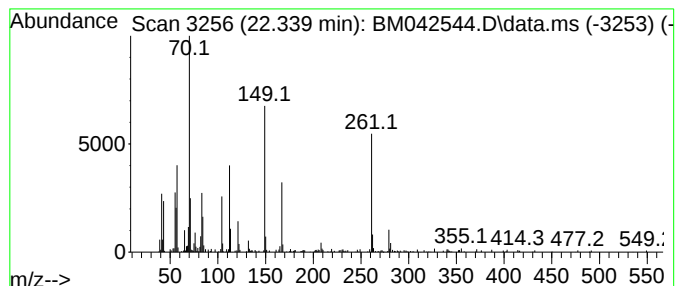
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.339	2.74 ng	218097	Chrysene-d12	21.503

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	70
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	49
3			Terephthalic acid, octyl 2,3,4-t...	408	C22H23F3O4	1010415-80-4	22
4			2-Ethylhexyl methacrylate	198	C12H22O2	000688-84-6	22
5			Terephthalic acid, 2-methylpent...	362	C22H34O4	1000356-19-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042544.D
Acq On : 01 Nov 2023 17:48
Operator : MA/JU
Sample : 05164-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI-352

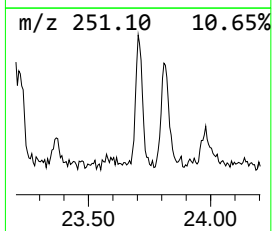
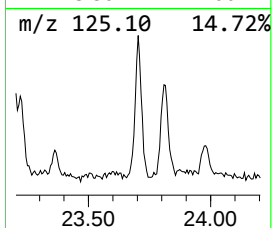
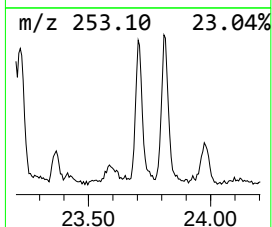
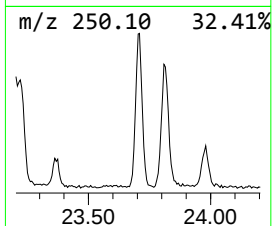
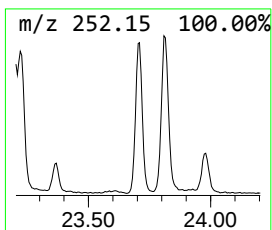
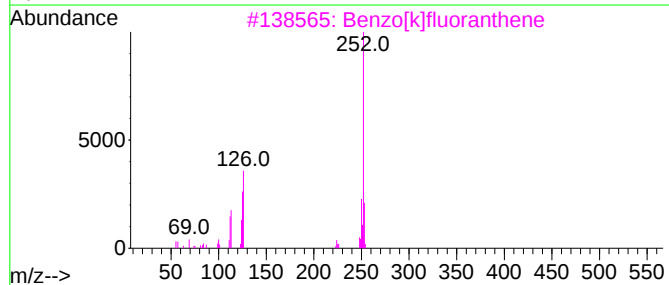
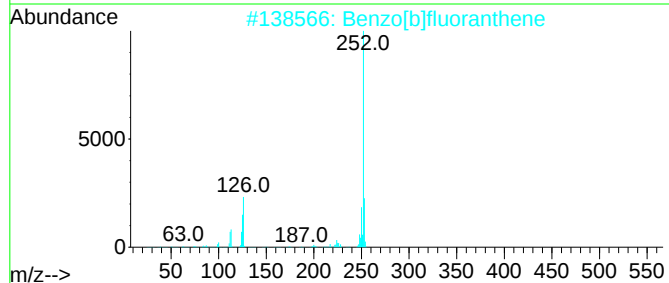
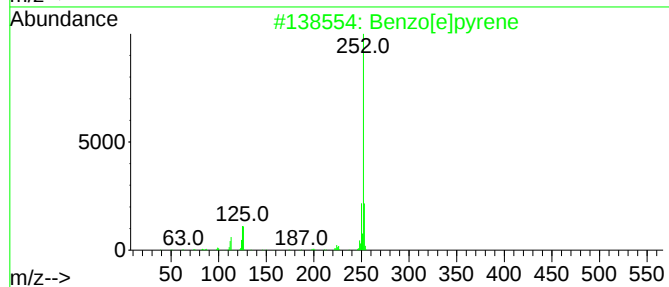
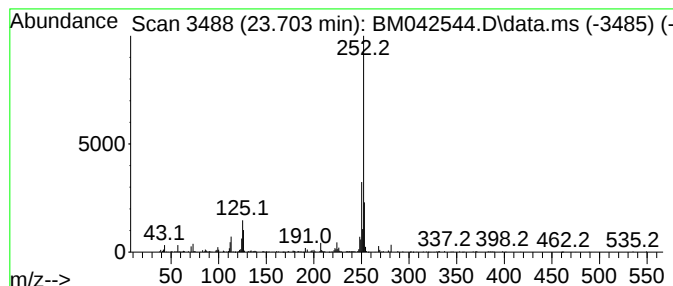
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
23.703	7.20 ng	404083	Perylene-d12	23.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Benzo[a]pyrene	252	C20H12	000050-32-8	94
5			Perylene	252	C20H12	000198-55-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042544.D
Acq On : 01 Nov 2023 17:48
Operator : MA/JU
Sample : 05164-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI-352

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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
2-Pentanone, 4-...	5.004	2.5	ng	69272	1	7.922	558897	20.0
2,4,7,9-Tetrame...	13.416	4.5	ng	216555	3	14.569	953771	20.0
n-Hexadecanoic ...	18.174	16.1	ng	931736	4	17.321	1157840	20.0
Octadecanoic acid	19.451	6.0	ng	481473	5	21.503	1593120	20.0
5-Eicosene, (E)-	21.168	8.0	ng	637816	5	21.503	1593120	20.0
1,4-Benzenedica...	22.339	2.7	ng	218097	5	21.503	1593120	20.0
Benzo[e]pyrene	23.703	7.2	ng	404083	6	23.927	1122550	20.0