

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111224\
 Data File : BE101584.D
 Acq On : 12 Nov 2024 16:01
 Operator : RC/JU
 Sample : P4796-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_E
 ClientSampleId :
 TP-3

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_E\Methods\8270-BE110624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BE101584.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.672	10	14	27	rBV	1688633	1941241	61.33%	12.903%
2	2.866	42	47	54	rBV	240456	302790	9.57%	2.013%
3	4.775	368	372	391	rBV	37213	64891	2.05%	0.431%
4	5.304	456	462	482	rBV	503544	836650	26.43%	5.561%
5	6.932	731	739	761	rBV	480375	915565	28.93%	6.085%
6	7.555	836	845	854	rBV	128765	207095	6.54%	1.376%
7	8.765	1042	1051	1067	rBV	325819	577238	18.24%	3.837%
8	10.322	1308	1316	1333	rBV	178570	332622	10.51%	2.211%
9	12.784	1727	1735	1759	rBV	1055514	1617375	51.10%	10.750%
10	14.164	1959	1970	1986	rBV	318633	502202	15.87%	3.338%
11	14.740	2059	2068	2083	rBV3	7365	37768	1.19%	0.251%
12	15.533	2197	2203	2217	rBV	131780	193893	6.13%	1.289%
13	15.669	2219	2226	2247	rBV	916086	1473011	46.54%	9.790%
14	16.902	2429	2436	2441	rBV	433507	642664	20.30%	4.272%
15	18.947	2779	2784	2795	rVB	53665	75166	2.37%	0.500%
16	19.317	2843	2847	2853	rVB	48266	64534	2.04%	0.429%
17	19.493	2871	2877	2888	rBV	2473742	3165235	100.00%	21.038%
18	21.062	3138	3144	3148	rBV	648922	838779	26.50%	5.575%
19	21.421	3202	3205	3210	rVB2	26548	32631	1.03%	0.217%
20	21.738	3255	3259	3265	rVB	74725	93293	2.95%	0.620%
21	22.314	3354	3357	3362	rVB	26916	35245	1.11%	0.234%
22	22.637	3408	3412	3416	rBV	30601	61610	1.95%	0.409%
23	23.342	3525	3532	3540	rBV	510504	1033885	32.66%	6.872%

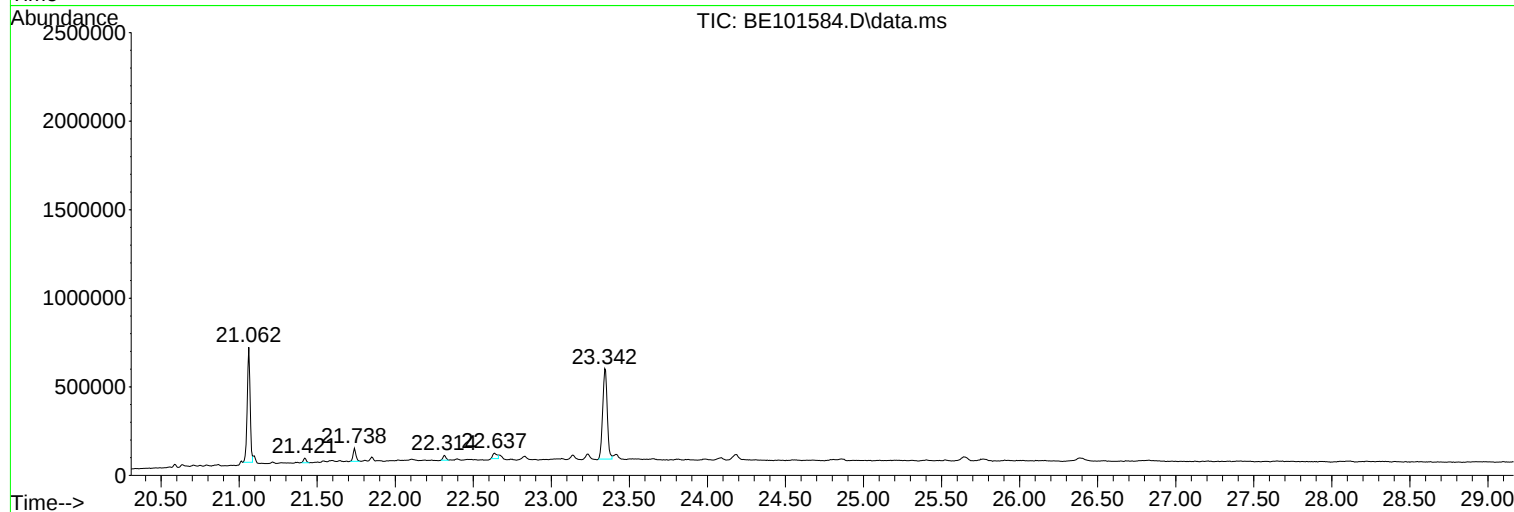
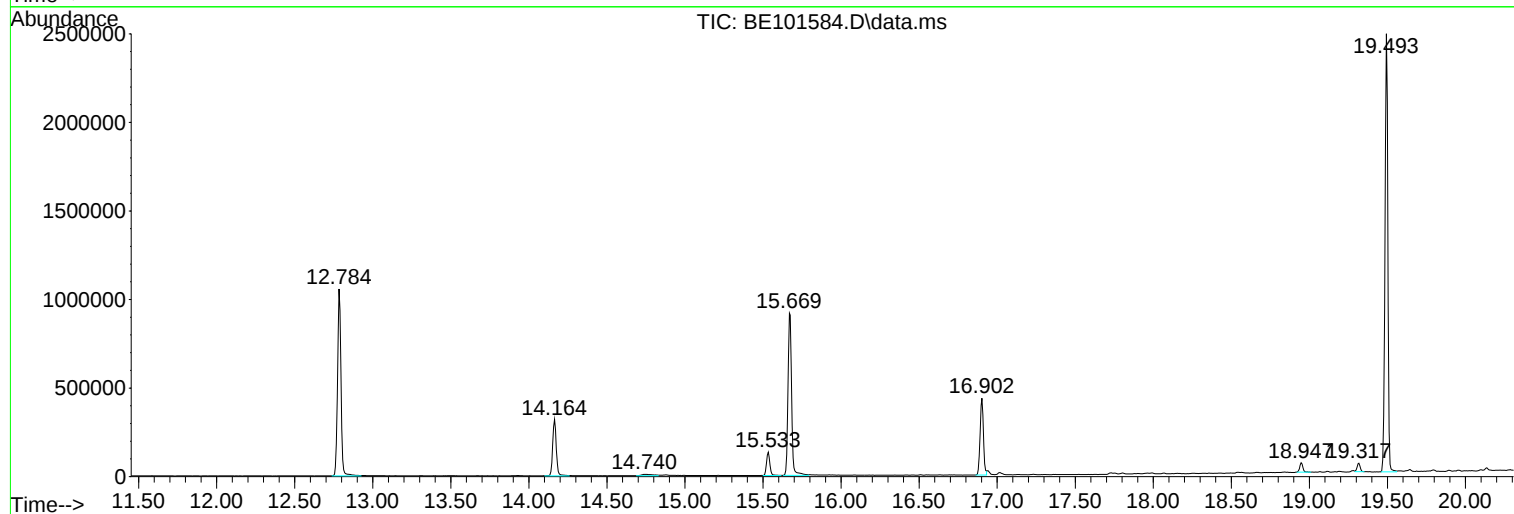
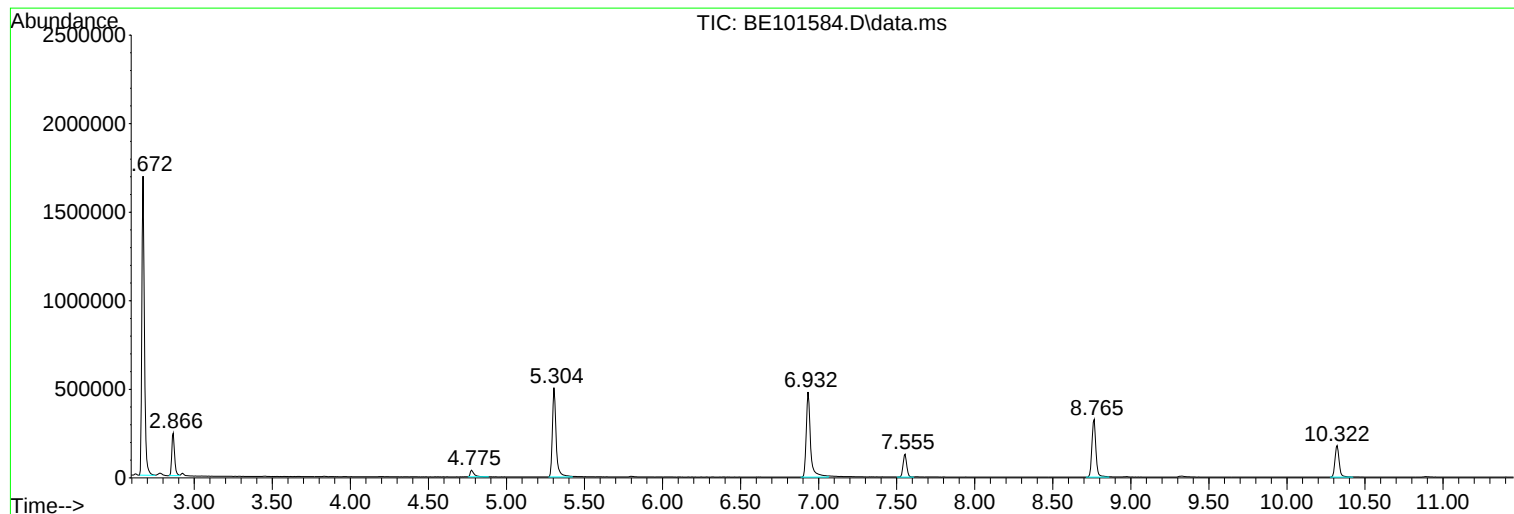
Sum of corrected areas: 15045383

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111224\
Data File : BE101584.D
Acq On : 12 Nov 2024 16:01
Operator : RC/JU
Sample : P4796-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.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_E\Data\BE111224\
Data File : BE101584.D
Acq On : 12 Nov 2024 16:01
Operator : RC/JU
Sample : P4796-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-3

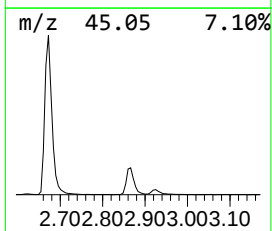
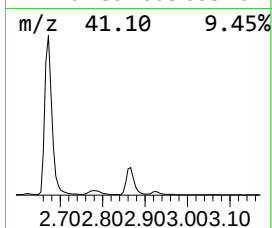
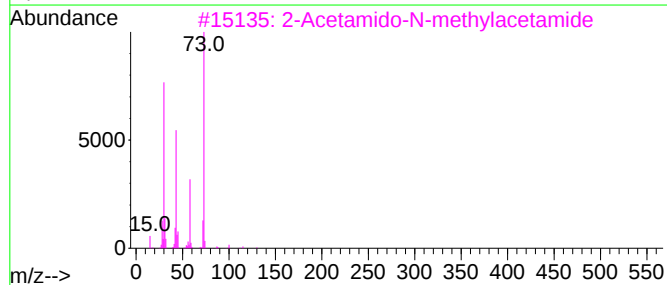
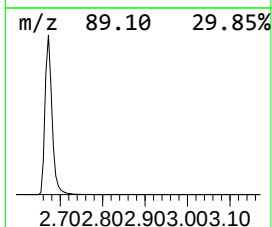
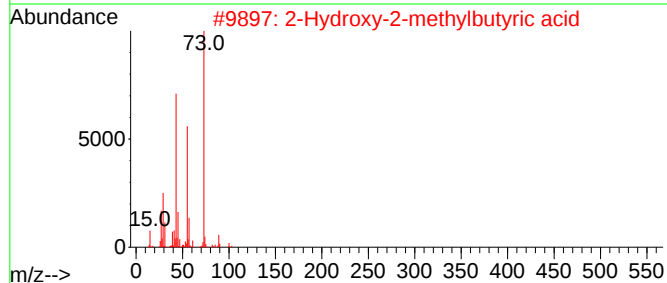
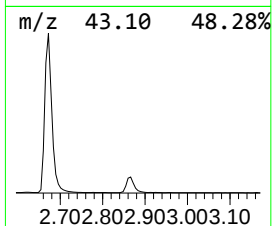
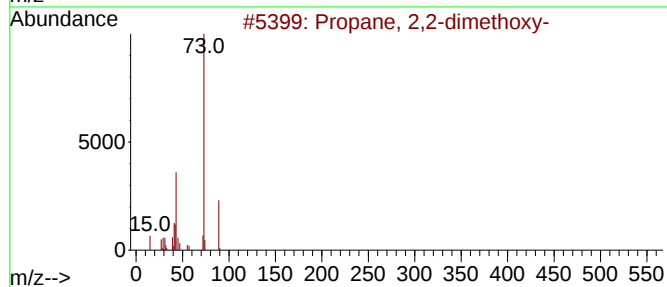
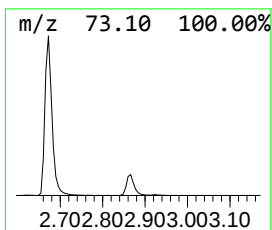
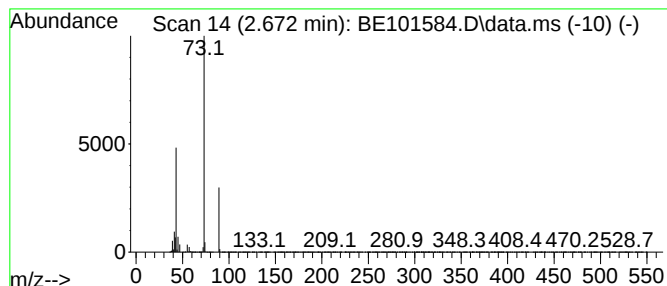
Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.672	187.47 ng	1941240	1,4-Dichlorobenzene-d4	7.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9
4			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5			1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111224\
Data File : BE101584.D
Acq On : 12 Nov 2024 16:01
Operator : RC/JU
Sample : P4796-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-3

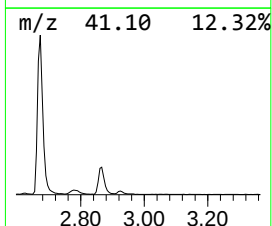
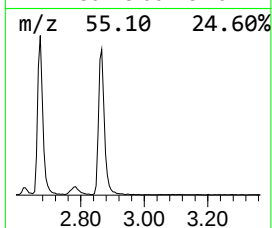
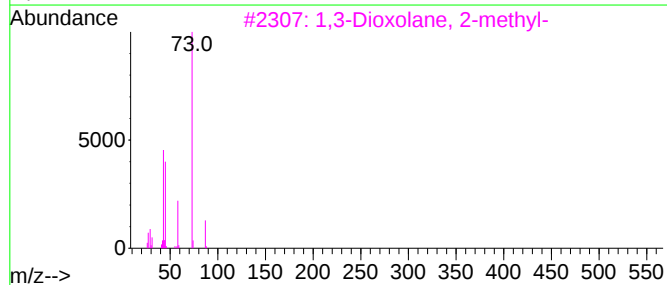
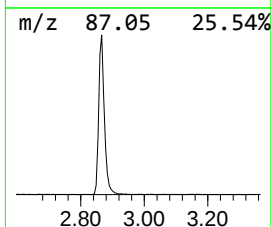
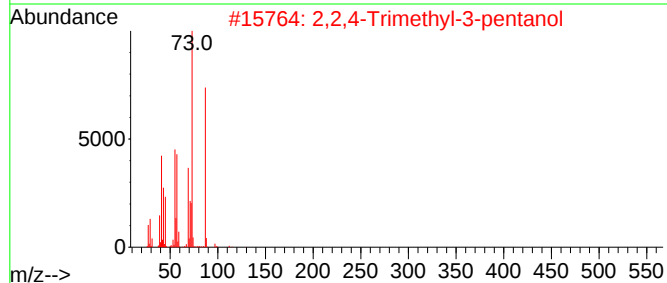
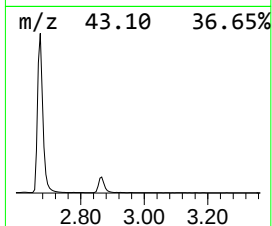
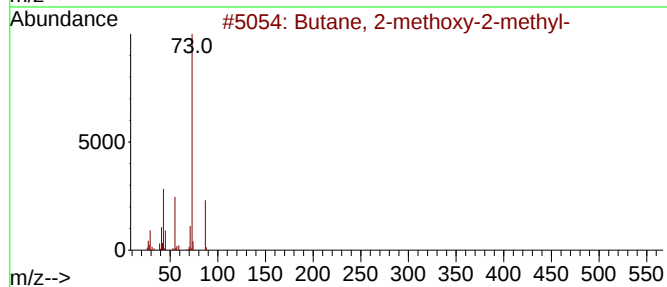
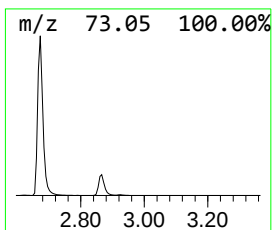
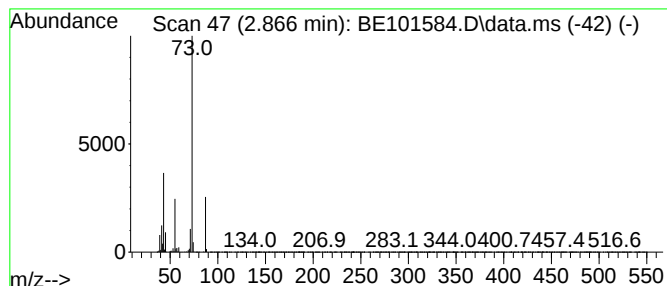
Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.866	29.24 ng	302790	1,4-Dichlorobenzene-d4	7.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111224\
Data File : BE101584.D
Acq On : 12 Nov 2024 16:01
Operator : RC/JU
Sample : P4796-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-3

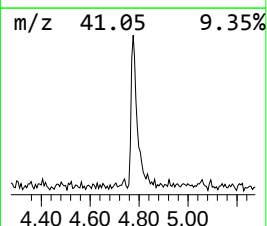
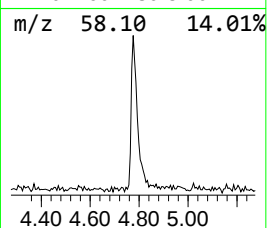
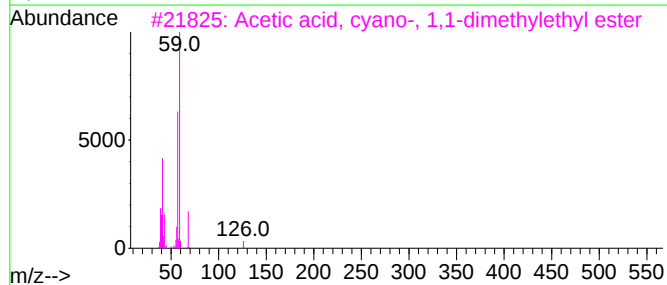
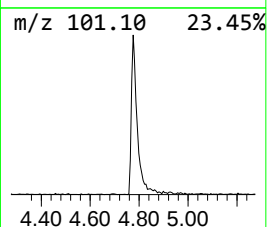
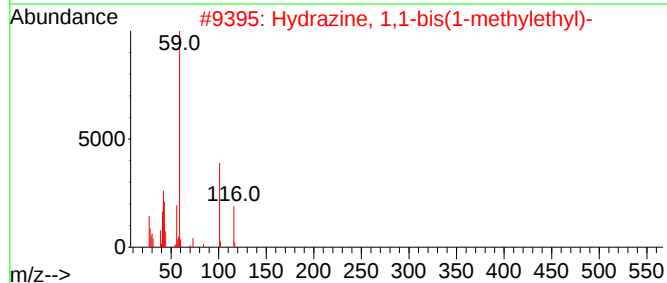
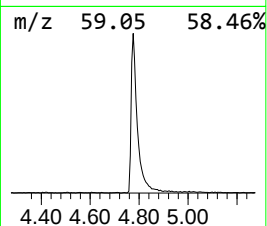
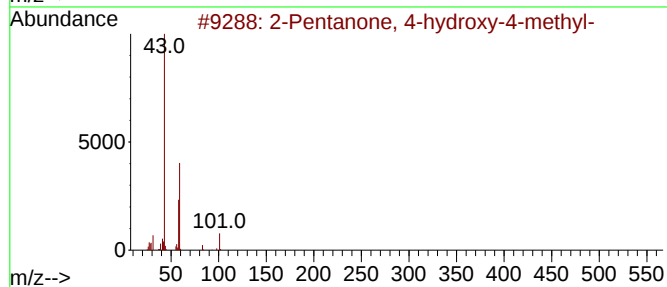
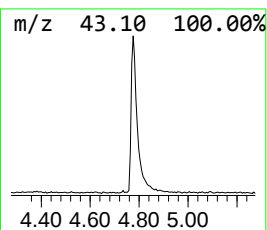
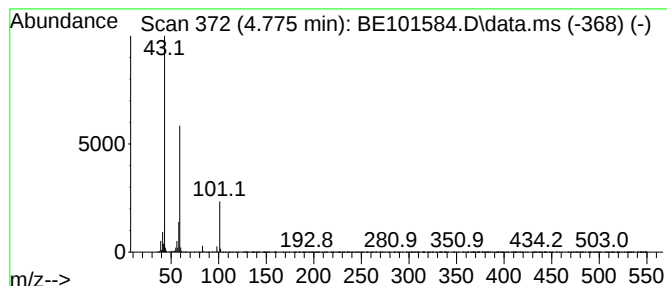
Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.775	6.27 ng	64891	1,4-Dichlorobenzene-d4	7.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			urea, N,N'-(dithiodi-2,1-ethane...	266	C8H18N4O2S2	1000401-66-6	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111224\
Data File : BE101584.D
Acq On : 12 Nov 2024 16:01
Operator : RC/JU
Sample : P4796-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-3

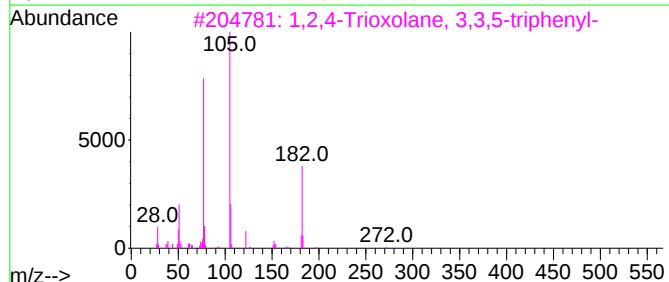
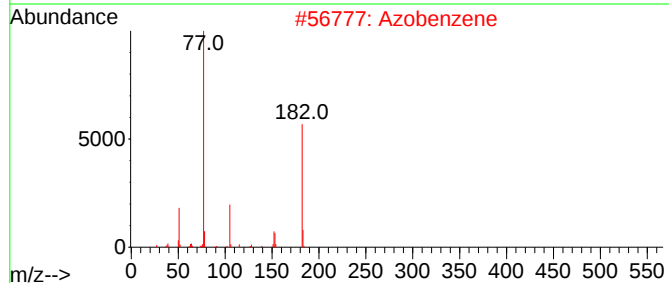
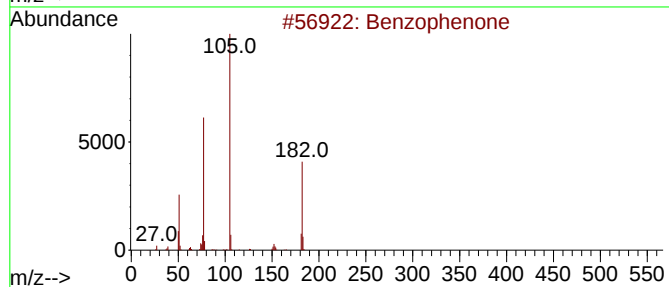
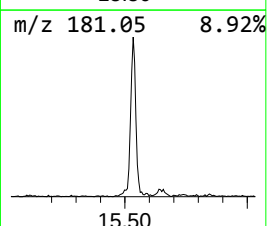
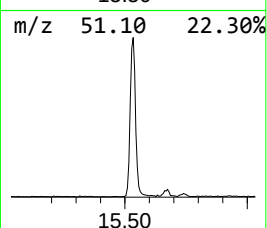
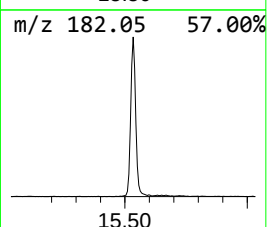
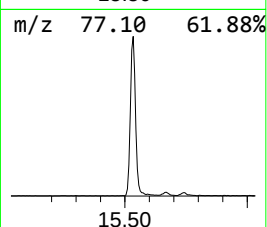
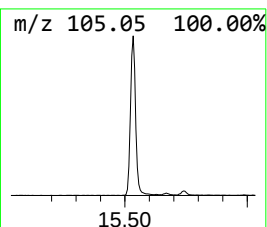
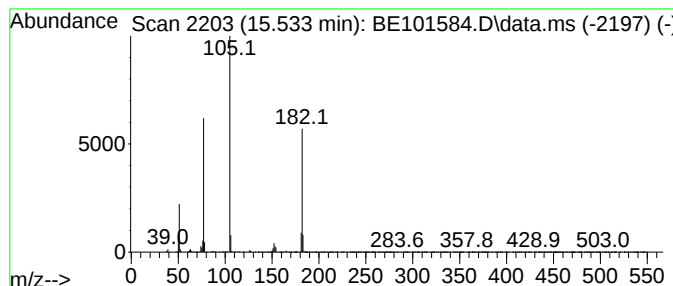
Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.533	7.72 ng	193893	Acenaphthene-d10	14.164

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	72
3			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
4			Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	45
5			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111224\
Data File : BE101584.D
Acq On : 12 Nov 2024 16:01
Operator : RC/JU
Sample : P4796-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-3

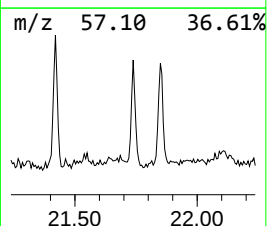
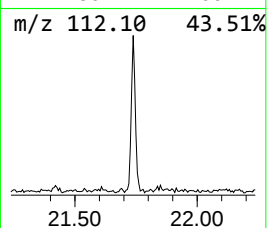
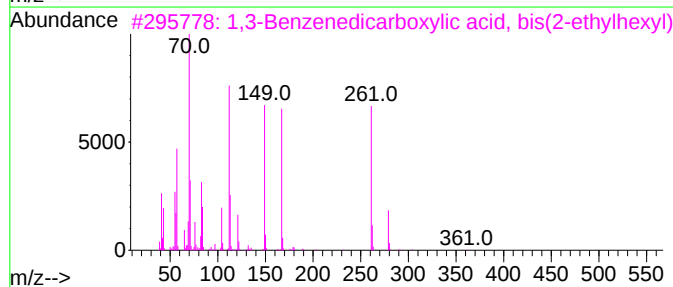
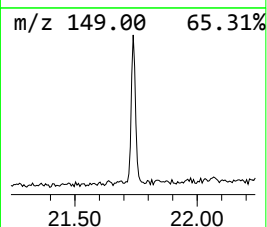
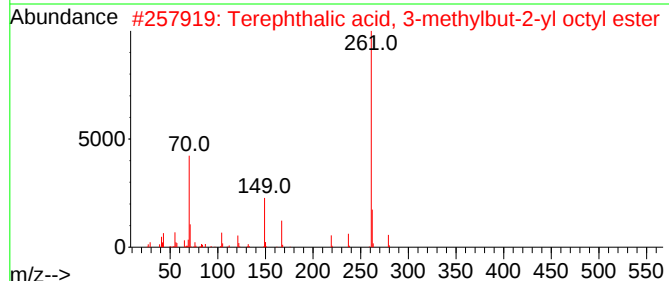
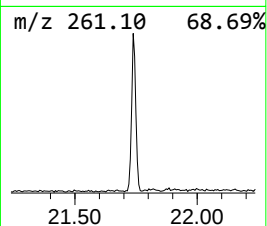
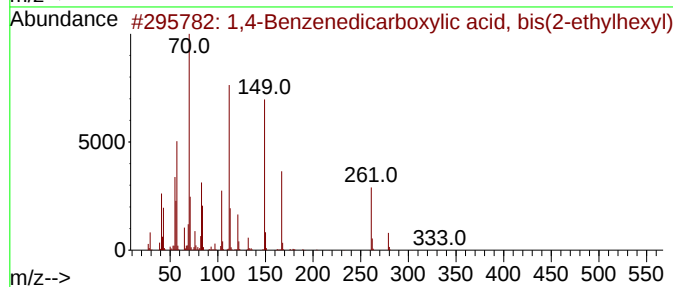
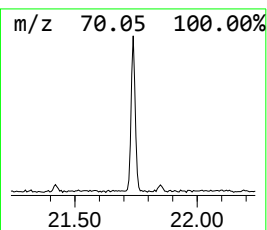
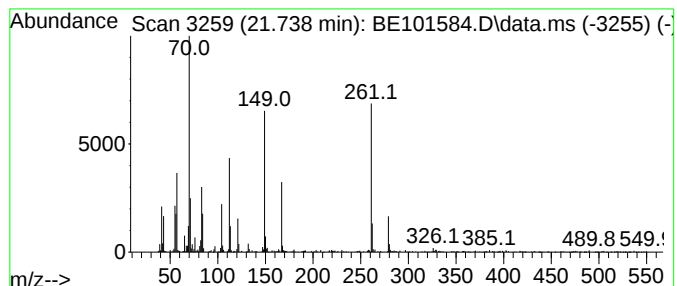
Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.738	2.22 ng	93293	Chrysene-d12	21.062

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	81
2			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	52
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
4			Terephthalic acid, 4-fluoro-2-me...	402	C23H27F05	1000415-83-4	38
5			Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111224\
Data File : BE101584.D
Acq On : 12 Nov 2024 16:01
Operator : RC/JU
Sample : P4796-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.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
Propane, 2,2-di...	2.672	187.5	ng	1941240	1	7.555	207095	20.0
Butane, 2-metho...	2.866	29.2	ng	302790	1	7.555	207095	20.0
2-Pentanone, 4-...	4.775	6.3	ng	64891	1	7.555	207095	20.0
Benzophenone	15.533	7.7	ng	193893	3	14.164	502202	20.0
1,4-Benzenedica...	21.738	2.2	ng	93293	5	21.062	838779	20.0