LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111124\
Data File : BE101573.D
Acq On : 11 Nov 2024 15:44
Operator : RC/JU
Sample : P4796-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-2

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: BE101573.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.670	10	14	28	rBV	1762723	1901644	54.51%	12.182%
2	2.864	43	47	54	rBV	256482	295118	8.46%	1.890%
3	4.774	368	372	392	rVB	36636	64102	1.84%	0.411%
4	5.303	456	462	486	rBV	486337	832080	23.85%	5.330%
5	6.936	732	740	775	rBV	447005	911456	26.13%	5.839%
6	7.553	838	845	854	rBV	135430	215876	6.19%	1.383%
7	8.763	1044	1051	1070	rBV	311096	544223	15.60%	3.486%
8	10.320	1309	1316	1328	rBV	184327	333675	9.57%	2.137%
9	12.788	1728	1736	1759	rBV	970166	1520521	43.59%	9.740%
10	14.163	1962	1970	1988	rBV	316507	509348	14.60%	3.263%
11	15.532	2198	2203	2216	rBV	118566	172172	4.94%	1.103%
12	15.673	2220	2227	2249	rBV	1009416	1522027	43.63%	9.750%
13	16.901	2429	2436	2450	rBV	485293	718170	20.59%	4.600%
14	19.498	2872	2878	2890	rBV	2731419	3488297	100.00%	22.345%
15	21.014	3133	3136	3139	rBV	31266	35147	1.01%	0.225%
16	21.067	3139	3145	3156	rVB	734983	974302	27.93%	6.241%
17	21.425	3202	3206	3212	rVB	36994	42311	1.21%	0.271%
18	21.742	3255	3260	3267	rBV	258369	320150	9.18%	2.051%
19	21.854	3276	3279	3283	rVB	32216	40112	1.15%	0.257%
20	22.318	3355	3358	3363	rVB	34358	47283	1.36%	0.303%
21	23.346	3526	3533	3542	rBV	554837	1122861	32.19%	7.193%

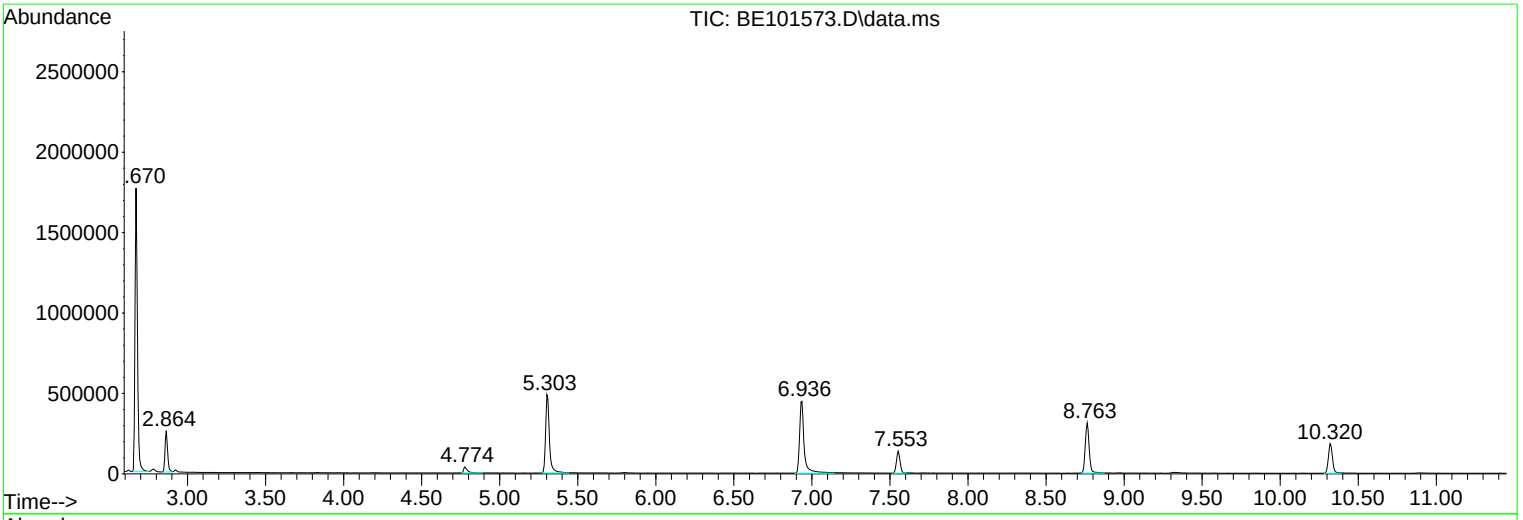
Sum of corrected areas: 15610875

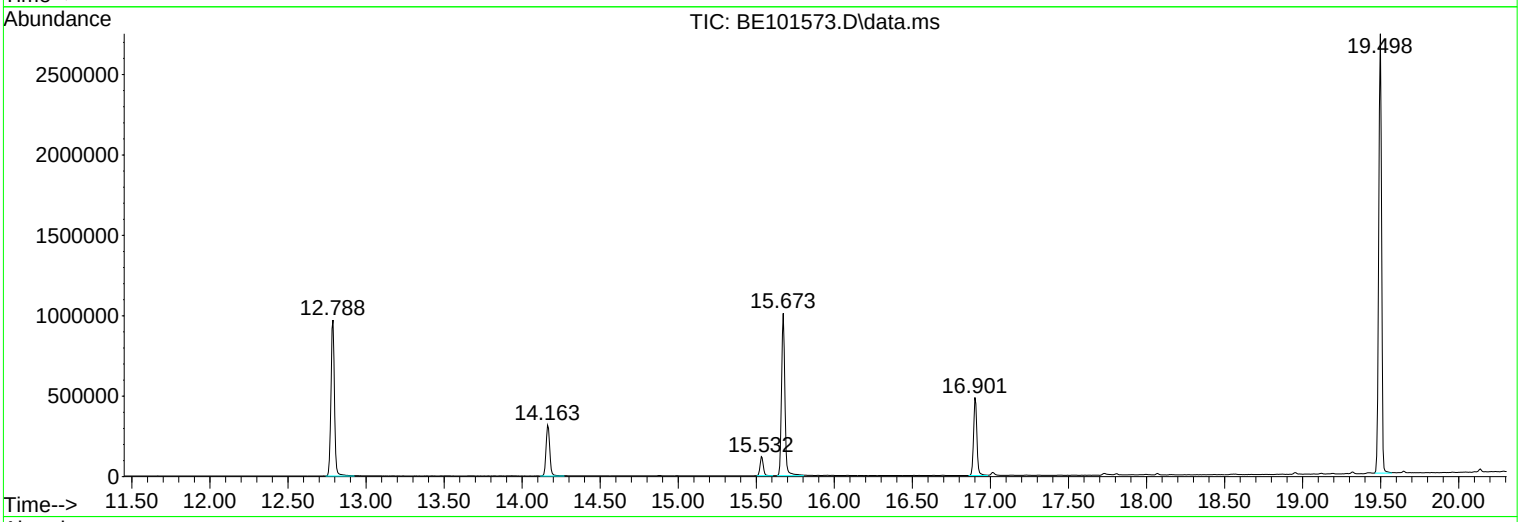
Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111124\
Data File : BE101573.D
Acq On : 11 Nov 2024 15:44
Operator : RC/JU
Sample : P4796-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

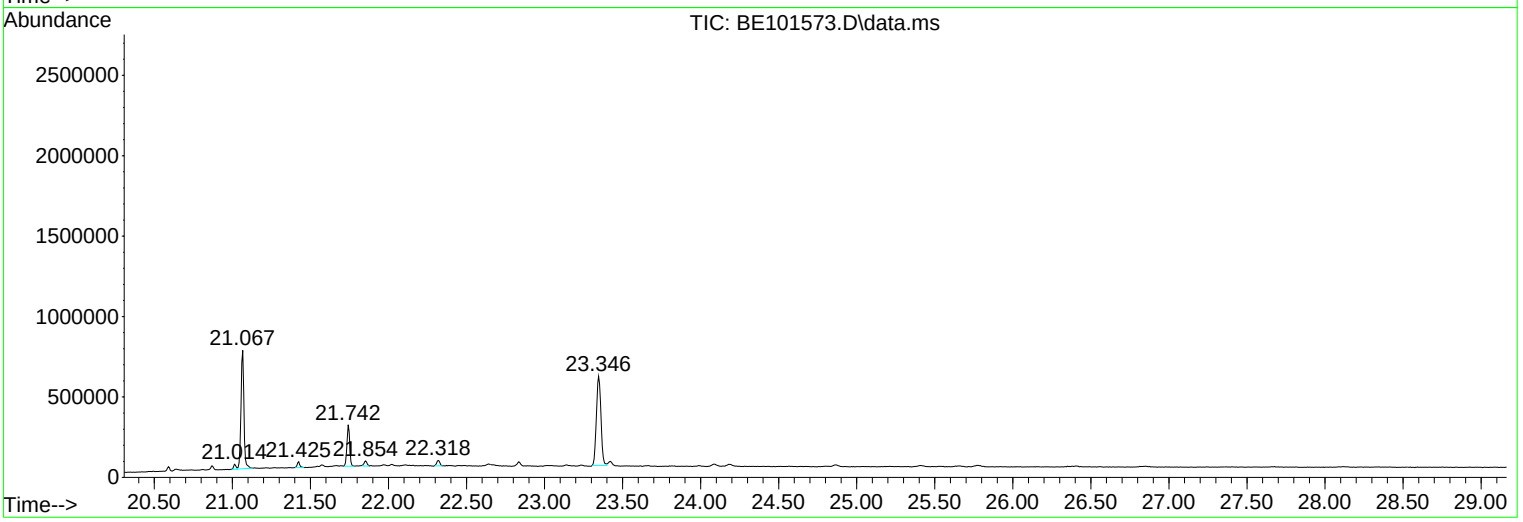
Instrument :
BNA_E
ClientSampleId :
TP-2

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\BE111124\
Data File : BE101573.D
Acq On : 11 Nov 2024 15:44
Operator : RC/JU
Sample : P4796-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-2

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

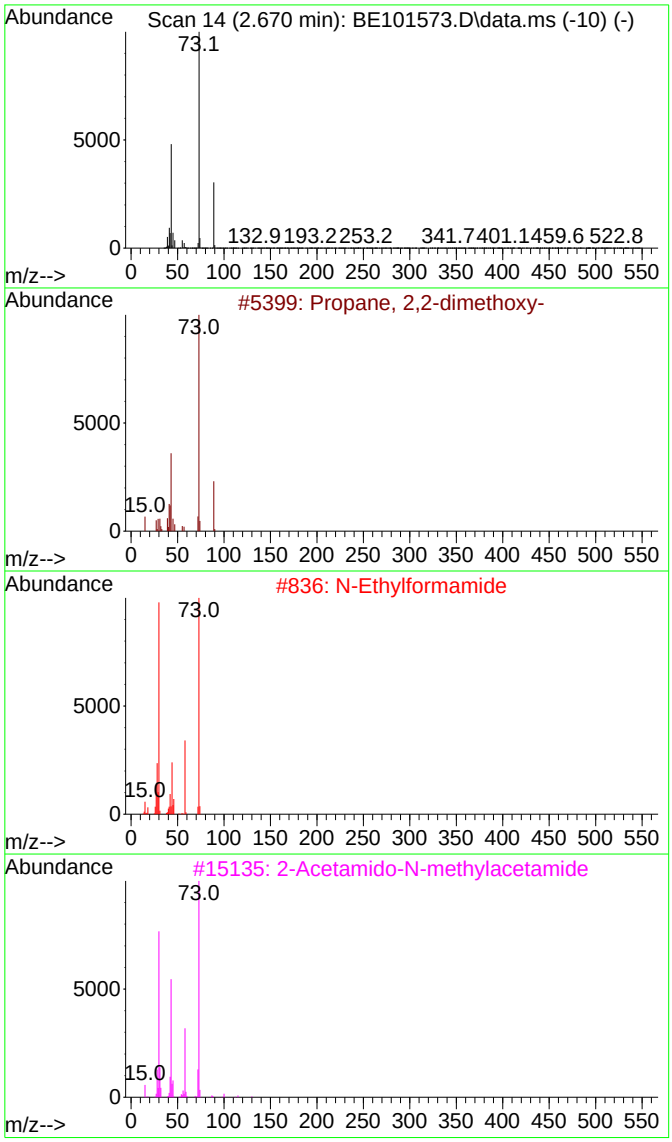
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

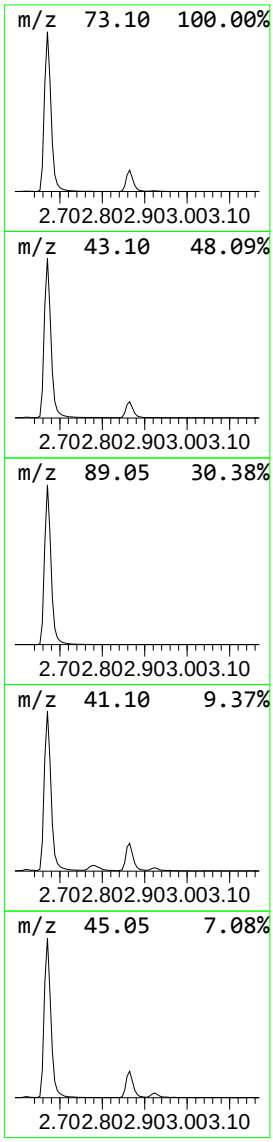
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.670	176.18 ng	1901640	1,4-Dichlorobenzene-d4	7.553

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	N-Ethylformamide	73	C3H7NO	000627-45-2	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	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111124\
Data File : BE101573.D
Acq On : 11 Nov 2024 15:44
Operator : RC/JU
Sample : P4796-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-2

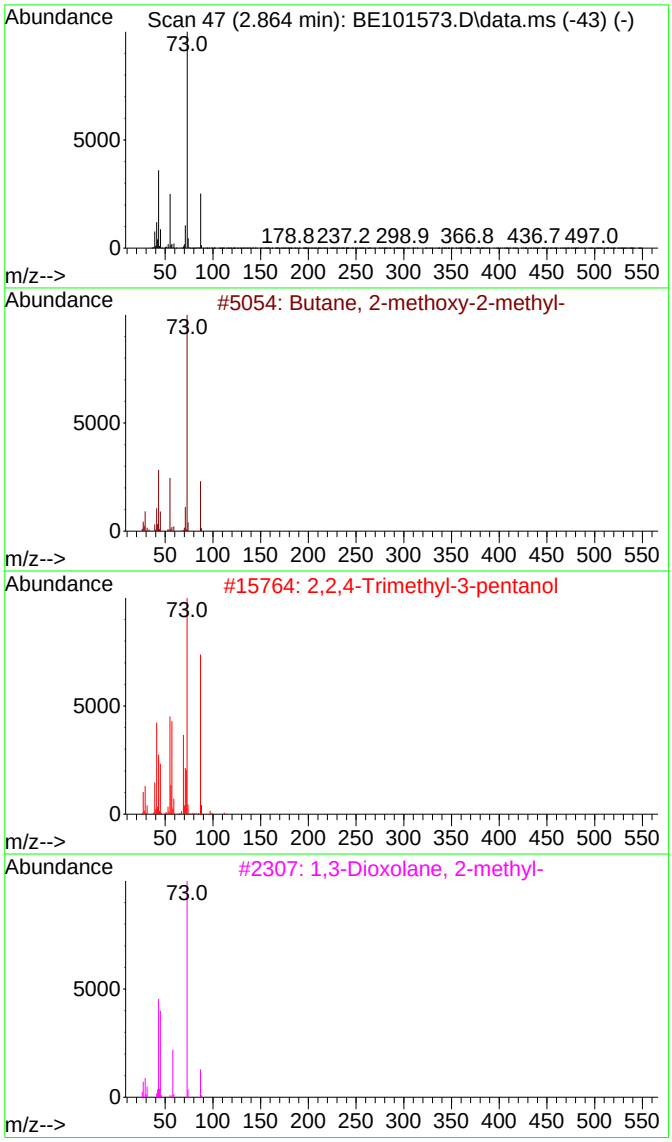
Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

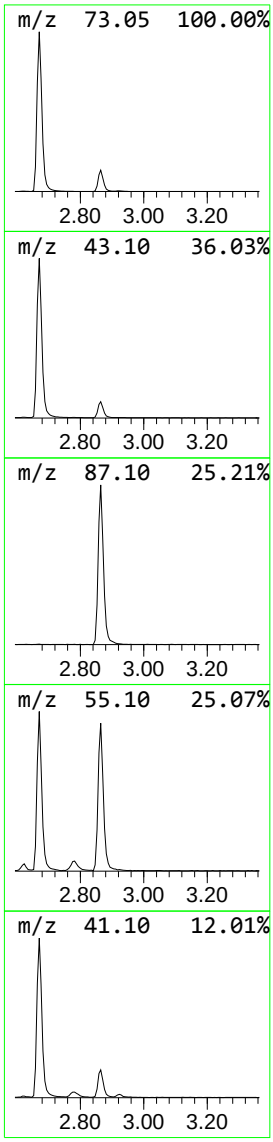
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.864	27.34 ng	295118	1,4-Dichlorobenzene-d4	7.553

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111124\
Data File : BE101573.D
Acq On : 11 Nov 2024 15:44
Operator : RC/JU
Sample : P4796-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-2

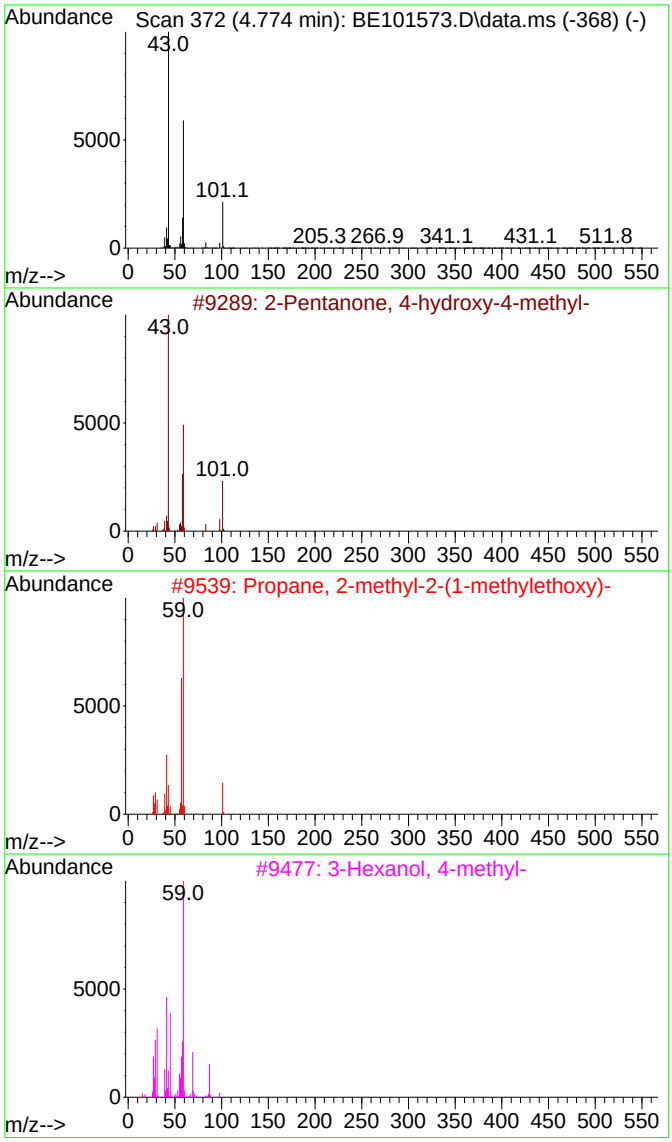
Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

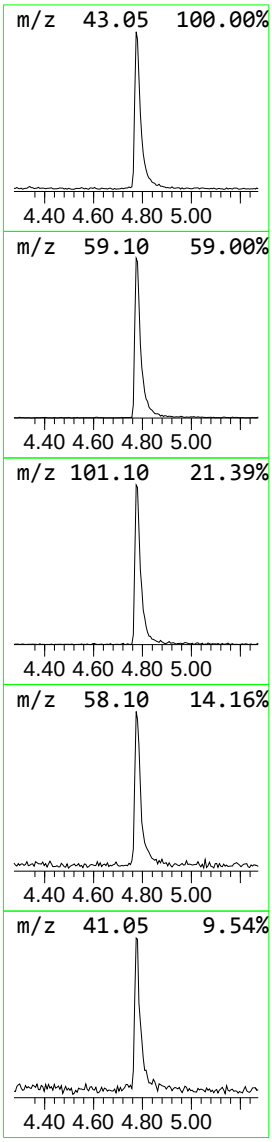
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.774	5.94 ng	64102	1,4-Dichlorobenzene-d4	7.553

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	Silane, trimethyl-	74	C3H10Si	000993-07-7	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111124\
Data File : BE101573.D
Acq On : 11 Nov 2024 15:44
Operator : RC/JU
Sample : P4796-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-2

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

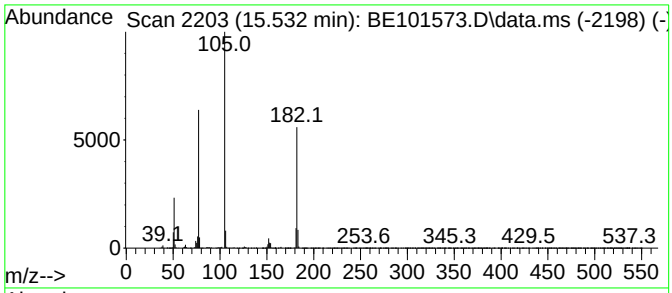
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

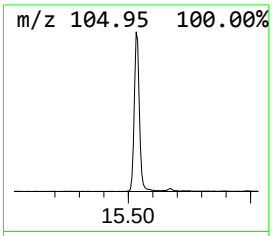
****

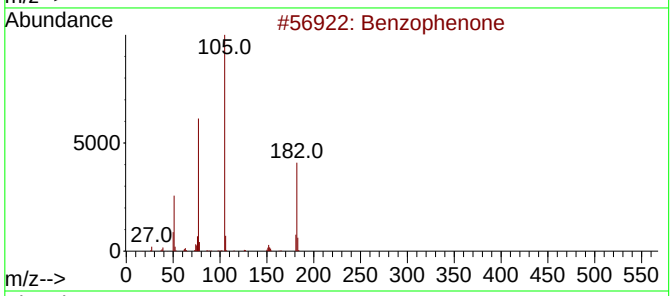
Peak Number 4 Benzophenone Concentration Rank 5

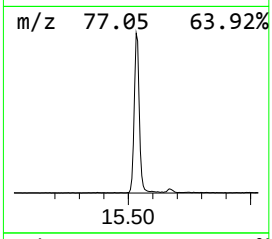
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.532	4.79 ng	172172	Phenanthrene-d10	16.901

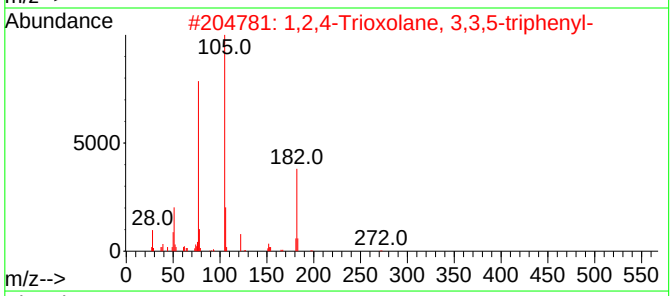
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
3	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	45
4	Azobenzene	182	C12H10N2	000103-33-3	42
5	Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	42

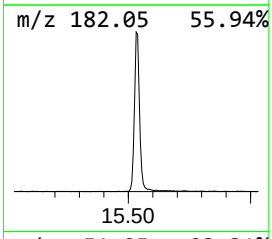


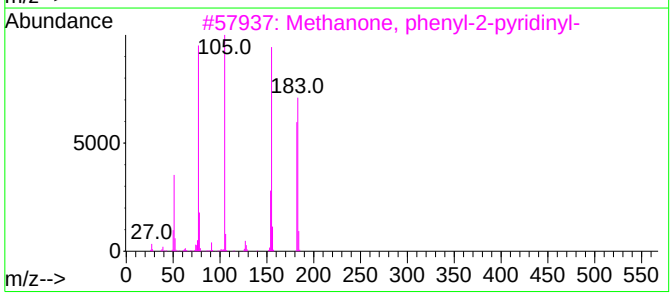


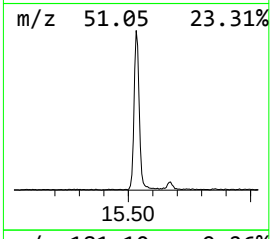


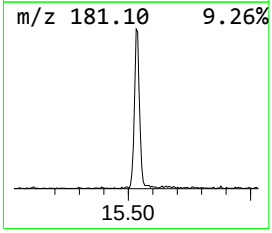












Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111124\
Data File : BE101573.D
Acq On : 11 Nov 2024 15:44
Operator : RC/JU
Sample : P4796-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-2

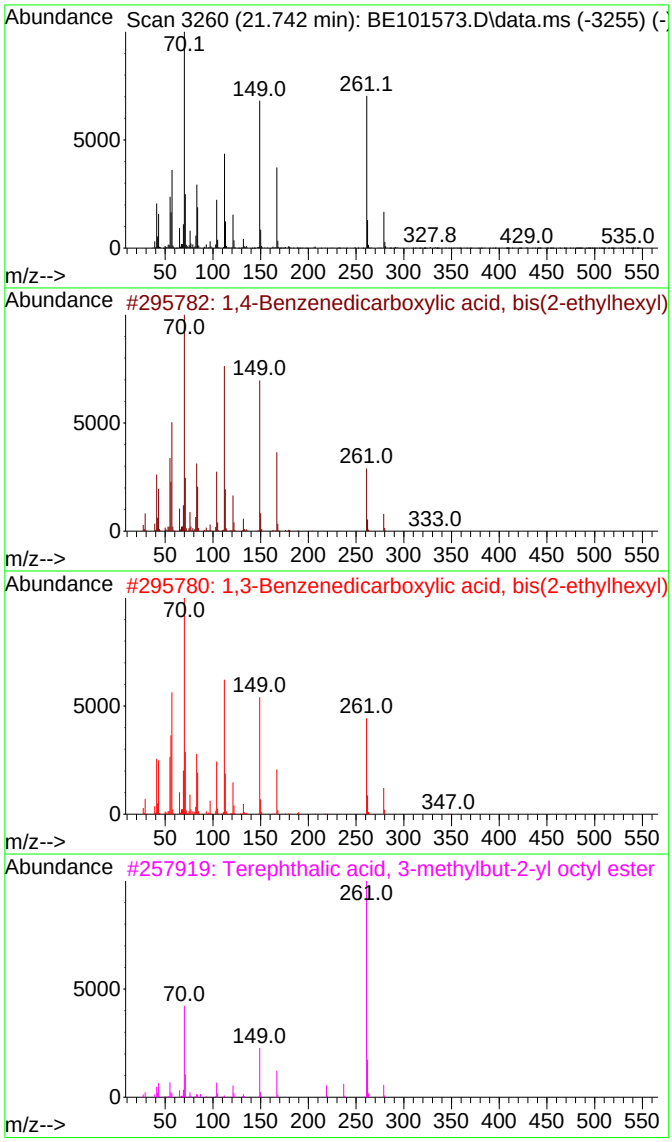
Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

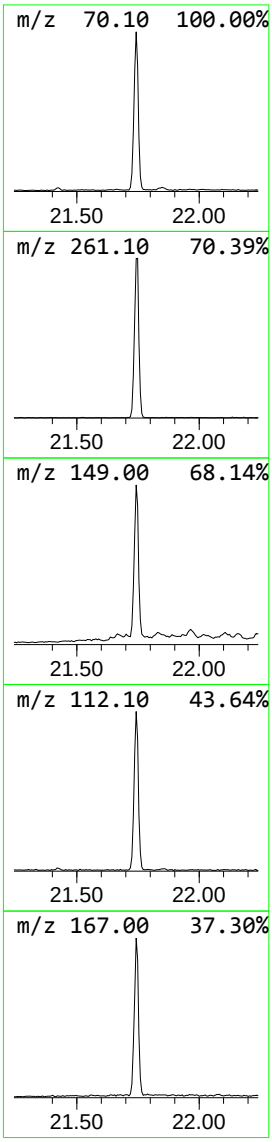
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.742	6.57 ng	320150	Chrysene-d12	21.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	74
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	52
4	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	38
5	Isophthalic acid, 3-methylbut-2-...	348	C21H32O4	1000344-72-4	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111124\
Data File : BE101573.D
Acq On : 11 Nov 2024 15:44
Operator : RC/JU
Sample : P4796-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
TP-2

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-di...	2.670	176.2	ng	1901640	1	7.553	215876	20.0
Butane, 2-metho...	2.864	27.3	ng	295118	1	7.553	215876	20.0
2-Pentanone, 4-...	4.774	5.9	ng	64102	1	7.553	215876	20.0
Benzophenone	15.532	4.8	ng	172172	4	16.901	718170	20.0
1,4-Benzenedica...	21.742	6.6	ng	320150	5	21.067	974302	20.0