LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049191.D
Acq On : 6 Jul 2021 18:54
Operator : CG/JU
Sample : M2926-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
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_G\METHODS\8270-BG063021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.126	9	15	24	rBV2	59625	141168	5.08%	1.008%
2	3.208	25	29	37	rVB2	31329	55347	1.99%	0.395%
3	5.165	357	362	368	rBV	18520	29176	1.05%	0.208%
4	5.641	436	443	456	rBV	778966	1342482	48.34%	9.581%
5	7.245	708	716	732	rBV	799450	1483507	53.42%	10.588%
6	7.374	732	738	745	rVB2	30922	58966	2.12%	0.421%
7	7.674	783	789	795	rBV2	17622	33883	1.22%	0.242%
8	8.085	852	859	866	rVB2	136824	236294	8.51%	1.686%
9	9.254	1047	1058	1068	rBV	502502	914945	32.95%	6.530%
10	10.905	1331	1339	1346	rBV	180038	332995	11.99%	2.377%
11	13.349	1747	1755	1764	rBV	1335253	2096842	75.50%	14.965%
12	14.172	1889	1895	1907	rVB	168065	250467	9.02%	1.788%
13	14.730	1983	1990	1997	rVB	283226	453918	16.34%	3.240%
14	16.217	2234	2243	2266	rBV	970241	1761534	63.43%	12.572%
15	17.480	2450	2458	2464	rBV	344456	536974	19.34%	3.832%
16	18.355	2603	2607	2613	rBV4	24237	41504	1.49%	0.296%
17	20.083	2895	2901	2909	rBV	2075726	2777113	100.00%	19.820%
18	21.393	3119	3124	3139	rBV2	143715	311651	11.22%	2.224%
19	21.757	3180	3186	3194	rBV2	322974	564485	20.33%	4.029%
20	21.910	3209	3212	3216	rVB6	22253	29148	1.05%	0.208%
21	25.065	3740	3749	3761	rVB2	185097	558971	20.13%	3.989%

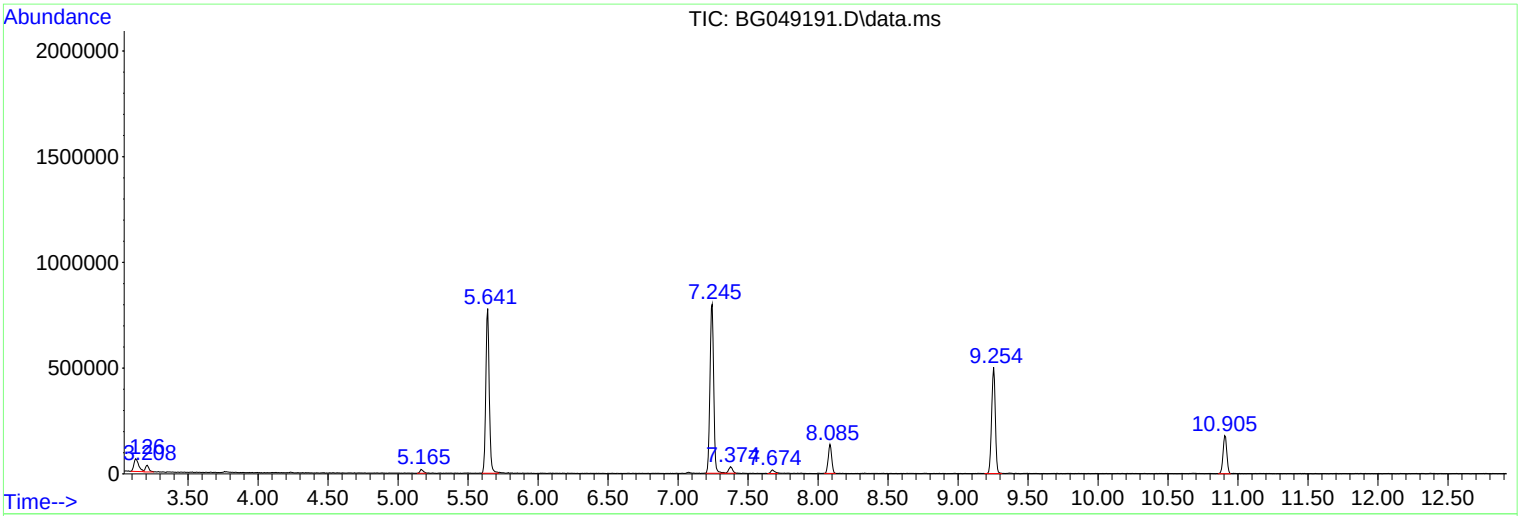
Sum of corrected areas: 14011370

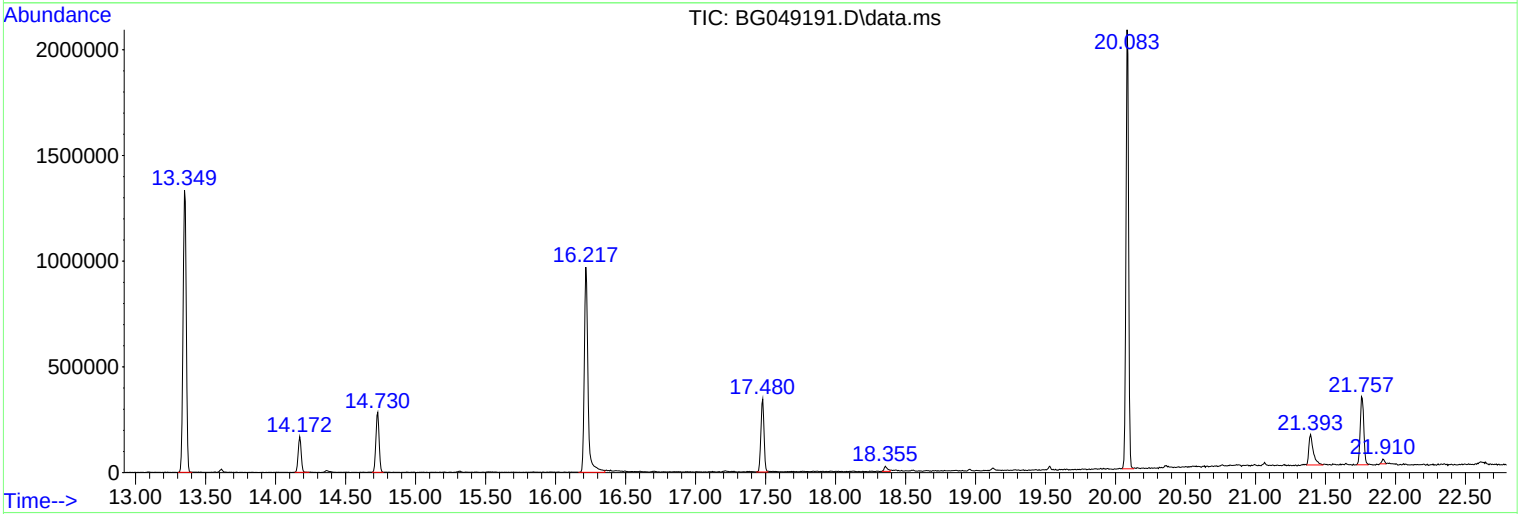
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049191.D
Acq On : 6 Jul 2021 18:54
Operator : CG/JU
Sample : M2926-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

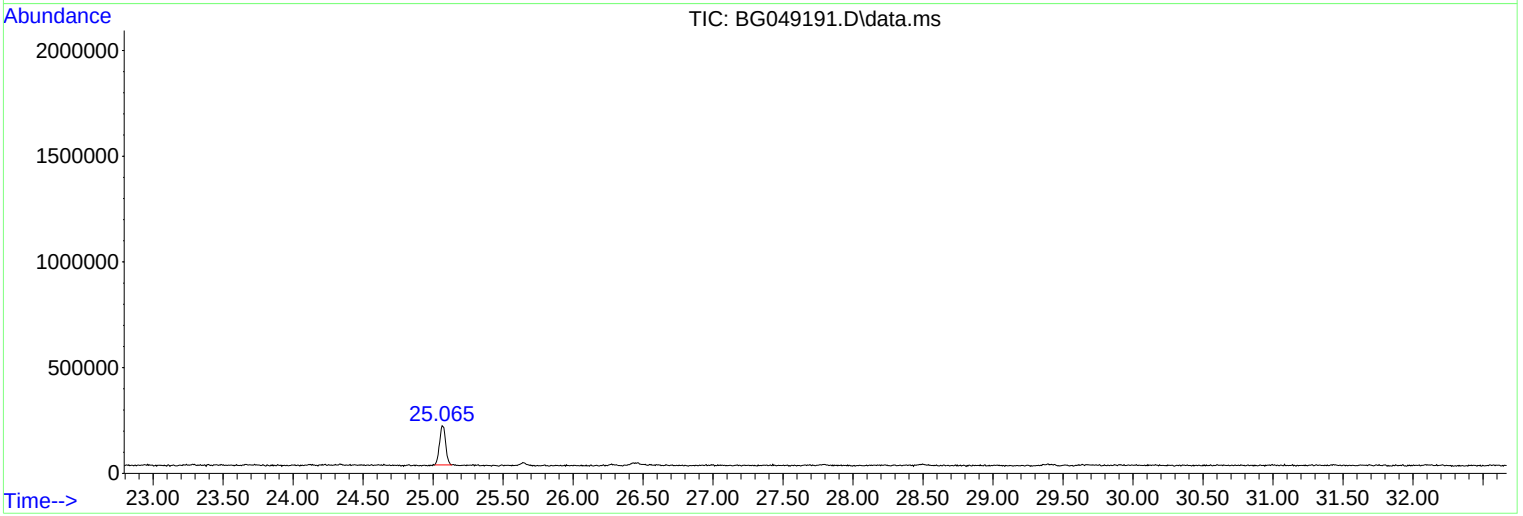
Instrument :
BNA_G
ClientSampleId :
TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.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_G\Data\BG070621\
Data File : BG049191.D
Acq On : 6 Jul 2021 18:54
Operator : CG/JU
Sample : M2926-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

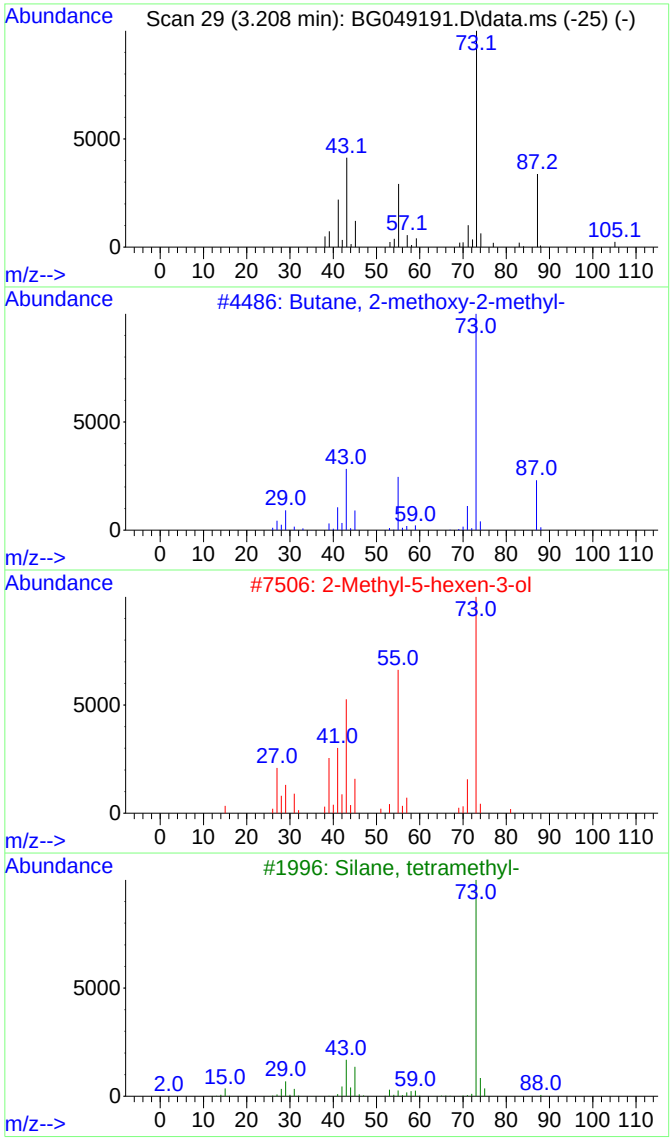
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

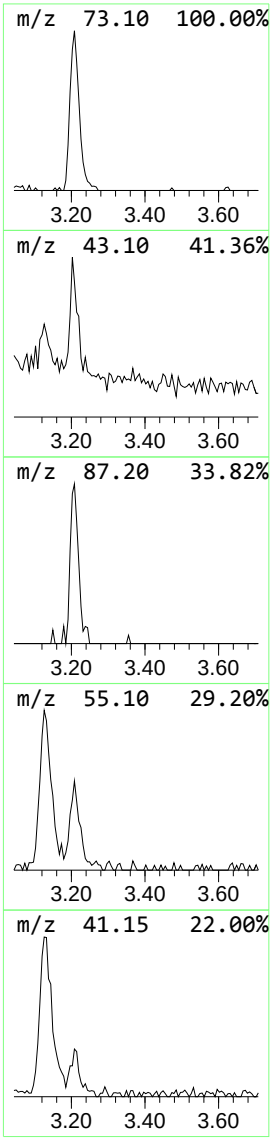
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.208	4.68 ng	55347	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	47
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049191.D
Acq On : 6 Jul 2021 18:54
Operator : CG/JU
Sample : M2926-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

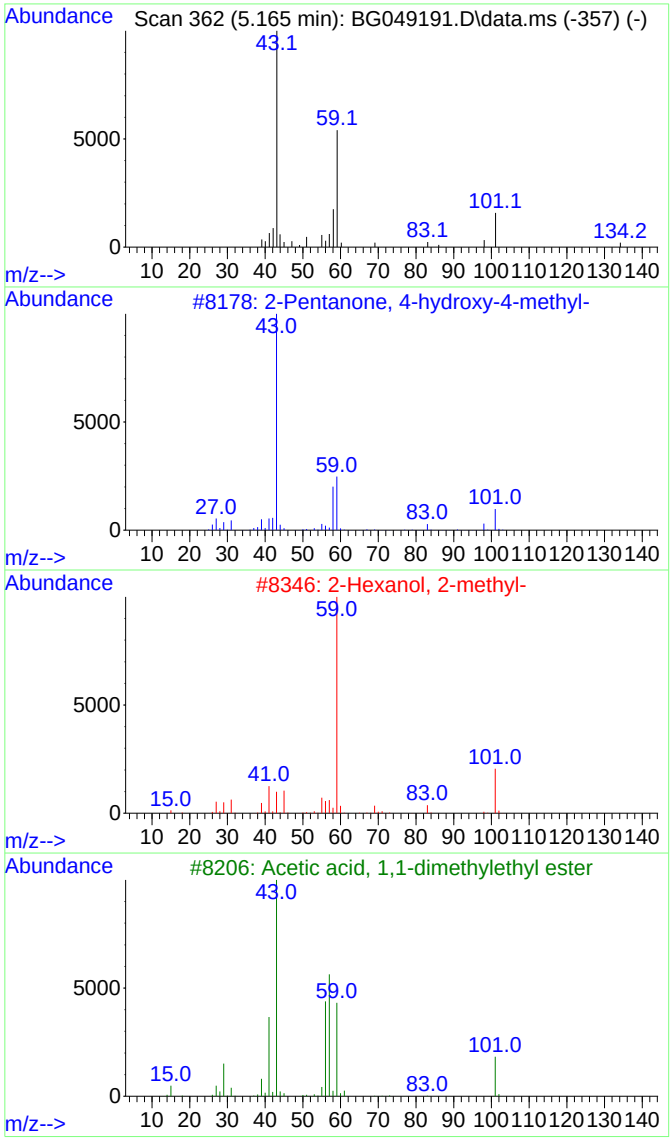
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

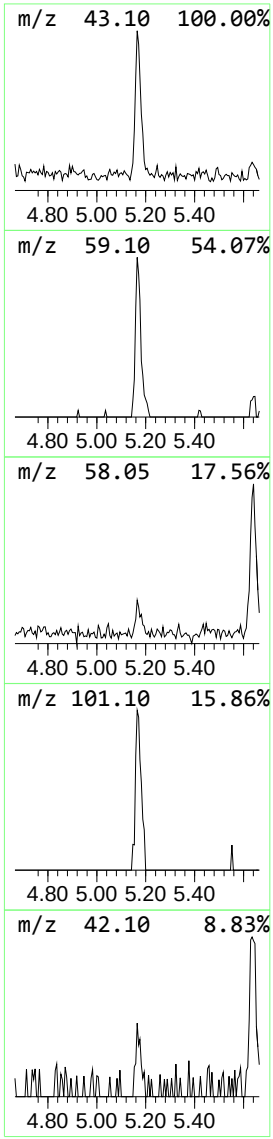
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.165	2.47 ng	29176	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	Diacetamide	101	C4H7NO2	000625-77-4	36
5	3-Hexanol	102	C6H14O	000623-37-0	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049191.D
Acq On : 6 Jul 2021 18:54
Operator : CG/JU
Sample : M2926-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

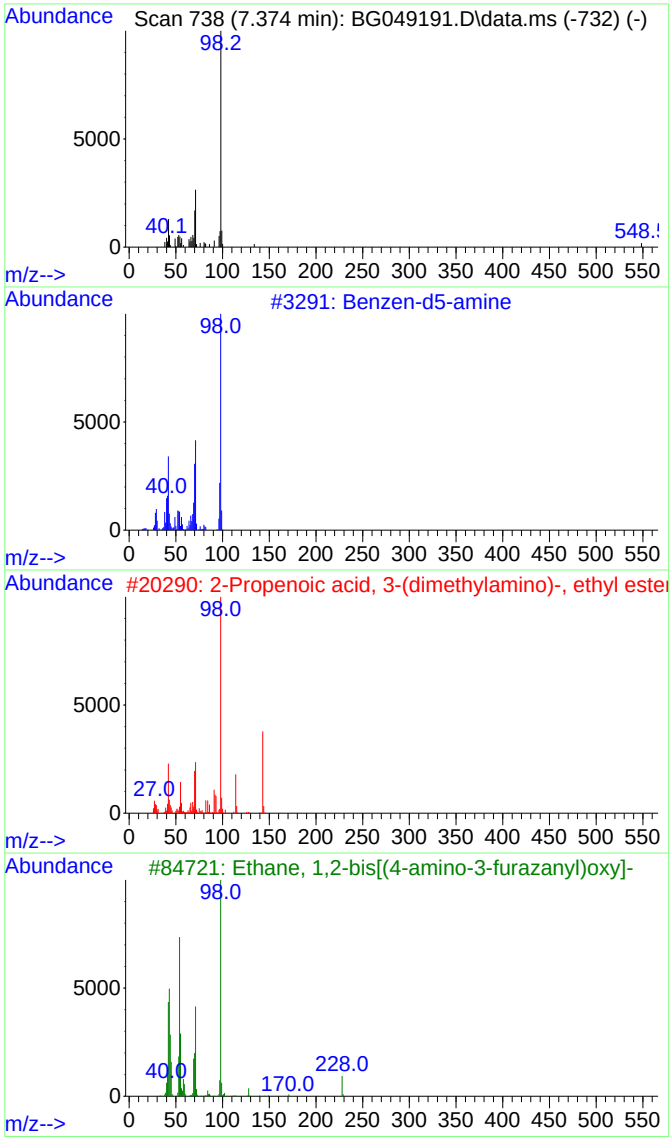
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

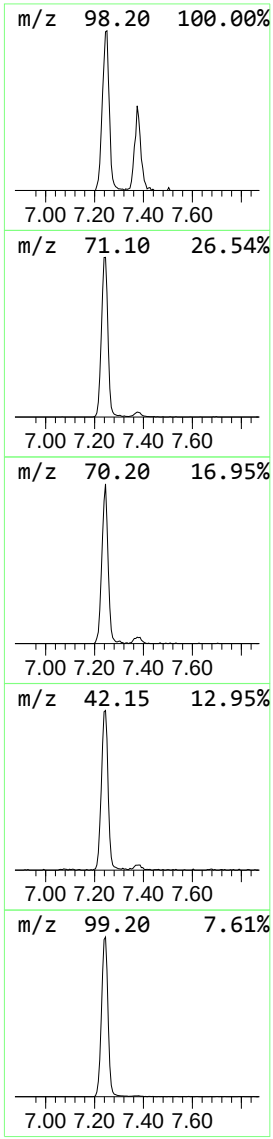
****

Peak Number 4 Benzen-d5-amine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.374	4.99 ng	58966	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzen-d5-amine	98	C6H2D5N	004165-61-1	86
2	2-Propenoic acid, 3-(dimethylami...	143	C7H13NO2	000924-99-2	56
3	Ethane, 1,2-bis[(4-amino-3-furaz...	228	C6H8N6O4	1000296-83-7	56
4	2-Pyrrolidinemethanamine, 1-ethyl-	128	C7H16N2	026116-12-1	53
5	1-Piperidineethanol	129	C7H15NO	003040-44-6	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049191.D
Acq On : 6 Jul 2021 18:54
Operator : CG/JU
Sample : M2926-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

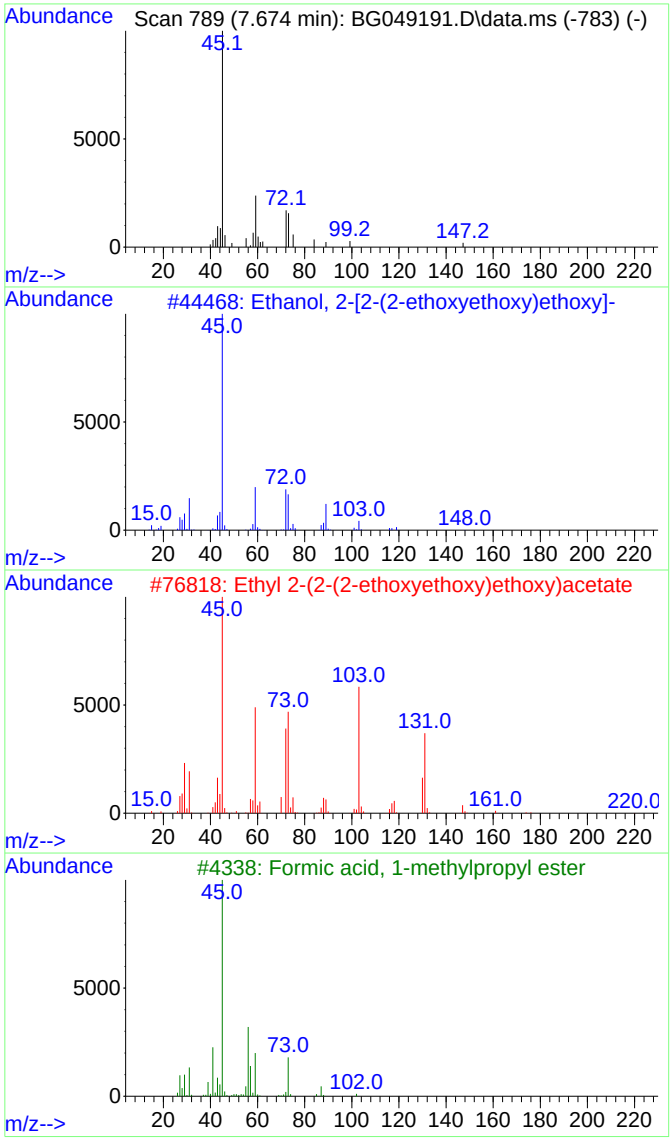
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

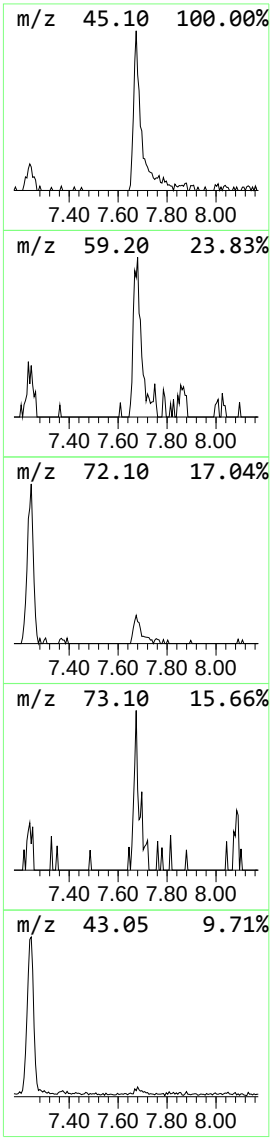
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-[2-(2-ethoxyetho... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.674	2.87 ng	33883	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	72
2	Ethyl 2-(2-(2-ethoxyethoxy)ethox...	220	C10H20O5	1000366-77-8	56
3	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	39
4	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	38
5	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049191.D
Acq On : 6 Jul 2021 18:54
Operator : CG/JU
Sample : M2926-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

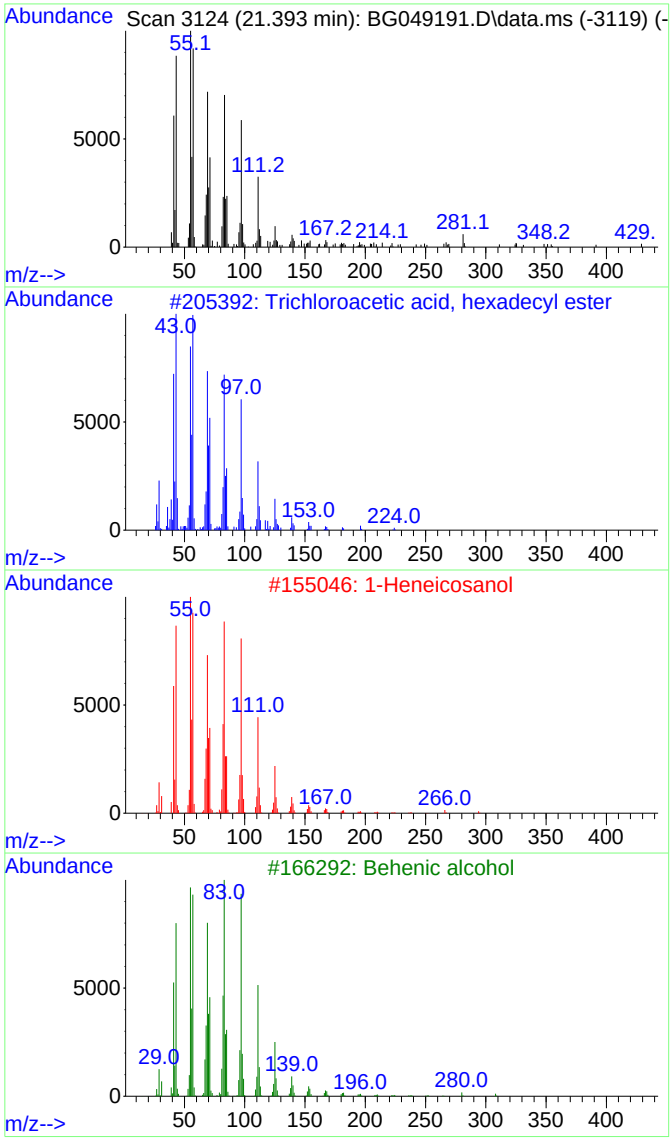
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

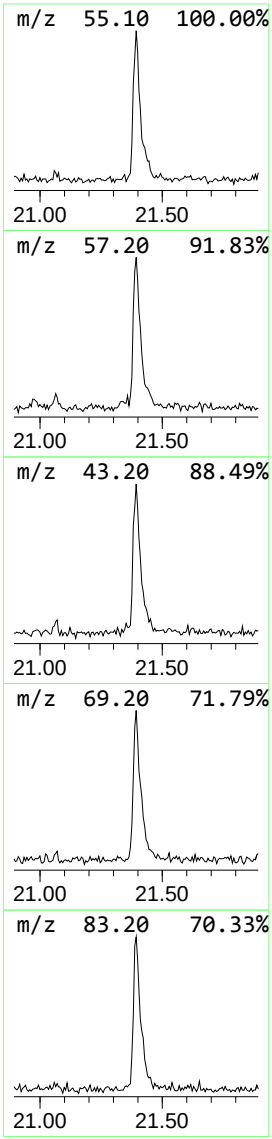
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.393	11.04 ng	311651	Chrysene-d12	21.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	1-Docosene	308	C22H44	001599-67-3	90
5	Cyclooctacosane	392	C28H56	000297-24-5	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049191.D
Acq On : 6 Jul 2021 18:54
Operator : CG/JU
Sample : M2926-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.208	4.7	ng	55347	1	8.085	236294	20.0
2-Pentanone, 4-...	5.165	2.5	ng	29176	1	8.085	236294	20.0
Benzen-d5-amine	7.374	5.0	ng	58966	1	8.085	236294	20.0
Ethanol, 2-[2-(...	7.674	2.9	ng	33883	1	8.085	236294	20.0
Trichloroacetic...	21.393	11.0	ng	311651	5	21.757	564485	20.0