LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061227.D
Acq On : 16 May 2024 19:23
Operator : MA/JU
Sample : P2480-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-MH-JJ

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-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061227.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.075	9	15	22	rVB6	9028	20592	1.48%	0.269%
2	3.152	22	28	44	rVB	247714	404373	29.13%	5.287%
3	3.669	112	116	123	rBV	21851	33202	2.39%	0.434%
4	5.525	424	432	444	rBV	344751	526138	37.91%	6.880%
5	7.112	694	702	717	rBV	344271	609261	43.90%	7.967%
6	7.928	832	841	847	rVB	108280	173340	12.49%	2.267%
7	9.080	1030	1037	1045	rBV	218965	389632	28.07%	5.095%
8	10.490	1272	1277	1284	rBV	23173	41115	2.96%	0.538%
9	10.719	1309	1316	1324	rBV	134468	241995	17.44%	3.164%
10	13.175	1726	1734	1741	rBV	591494	909872	65.56%	11.897%
11	14.556	1963	1969	1978	rVB	244512	365145	26.31%	4.775%
12	14.761	1999	2004	2005	rBV3	8884	13981	1.01%	0.183%
13	16.048	2217	2223	2237	rBV	510696	805914	58.07%	10.538%
14	17.306	2428	2437	2447	rBV	302576	452101	32.57%	5.912%
15	17.693	2498	2503	2510	rBV7	9989	22149	1.60%	0.290%
16	18.204	2585	2590	2599	rBV2	30915	53409	3.85%	0.698%
17	19.920	2876	2882	2895	rBV	1009661	1387931	100.00%	18.148%
18	21.219	3099	3103	3113	rBV3	42732	85203	6.14%	1.114%
19	21.559	3156	3161	3169	rVB	301031	495414	35.69%	6.478%
20	23.204	3437	3441	3446	rVB	36311	60404	4.35%	0.790%
21	24.685	3684	3693	3709	rVB2	189136	556595	40.10%	7.278%

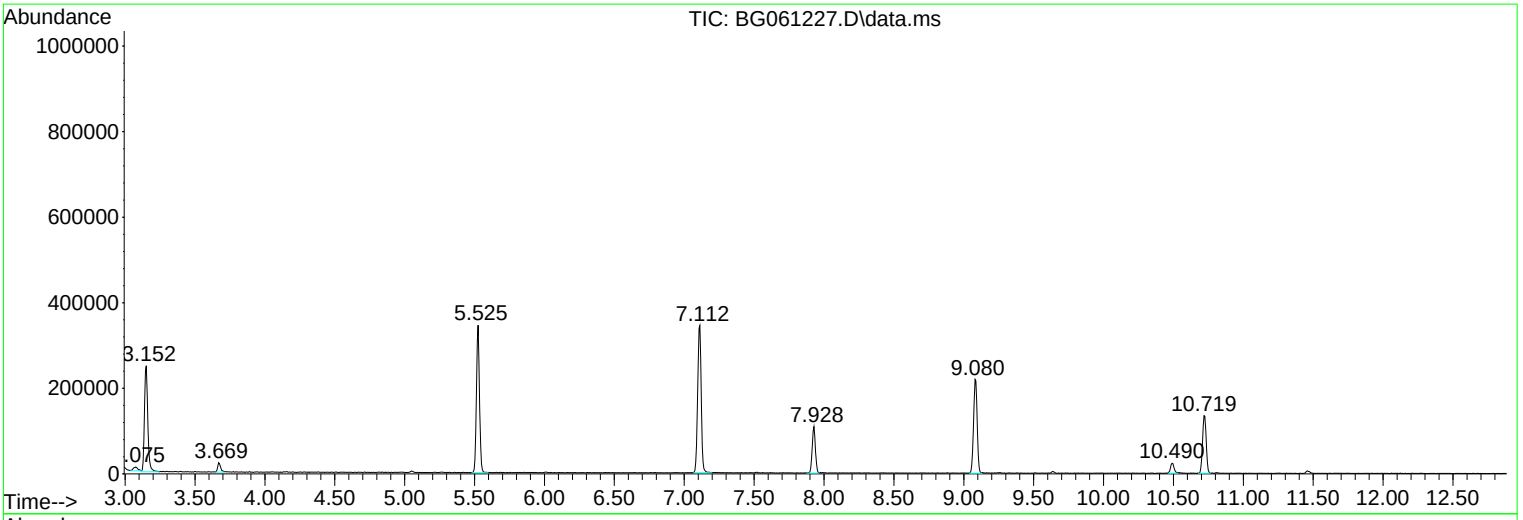
Sum of corrected areas: 7647766

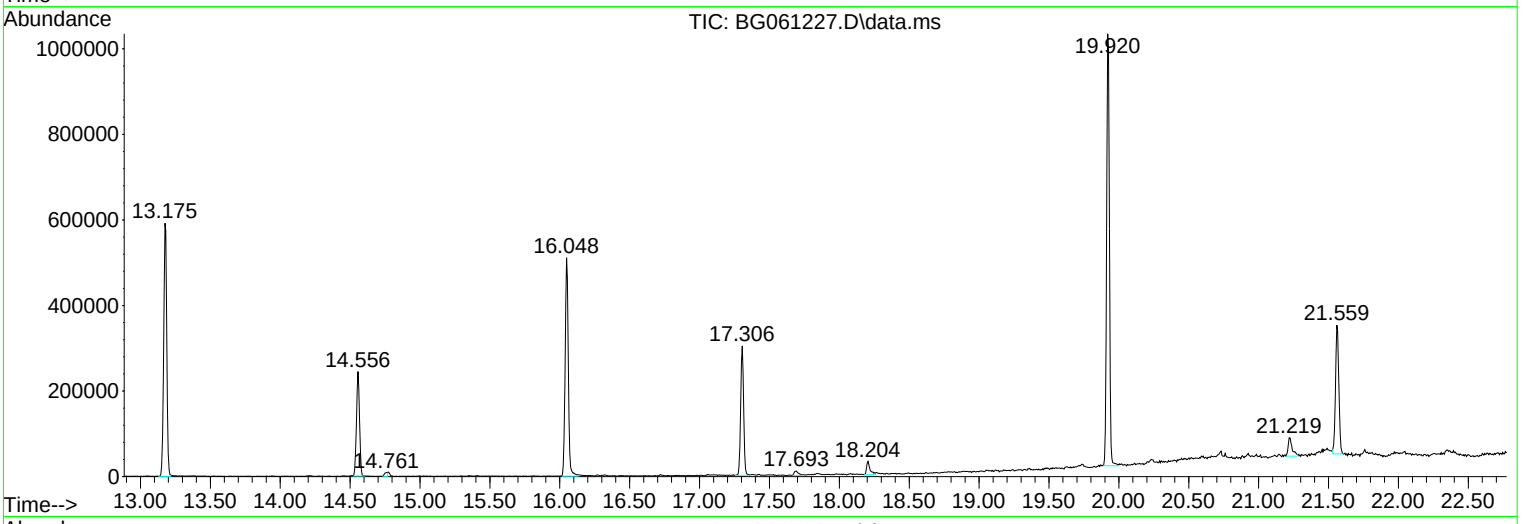
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061227.D
Acq On : 16 May 2024 19:23
Operator : MA/JU
Sample : P2480-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

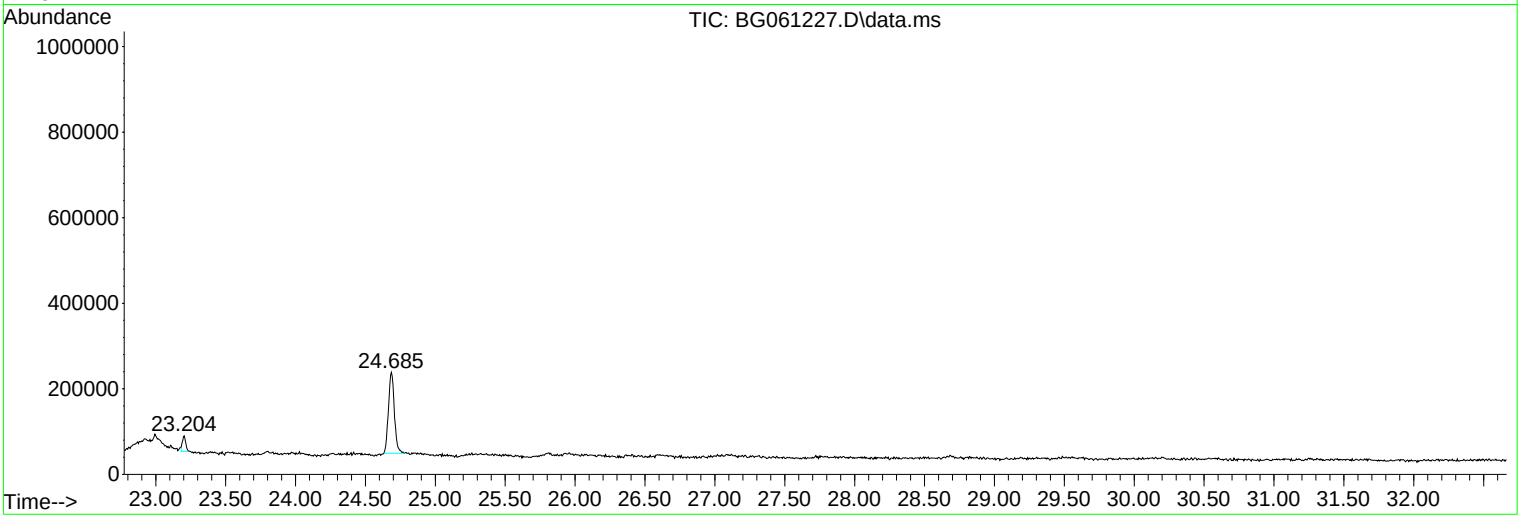
Instrument :
BNA_G
ClientSampleId :
WC-MH-JJ

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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_G\Data\BG051624\
Data File : BG061227.D
Acq On : 16 May 2024 19:23
Operator : MA/JU
Sample : P2480-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-MH-JJ

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

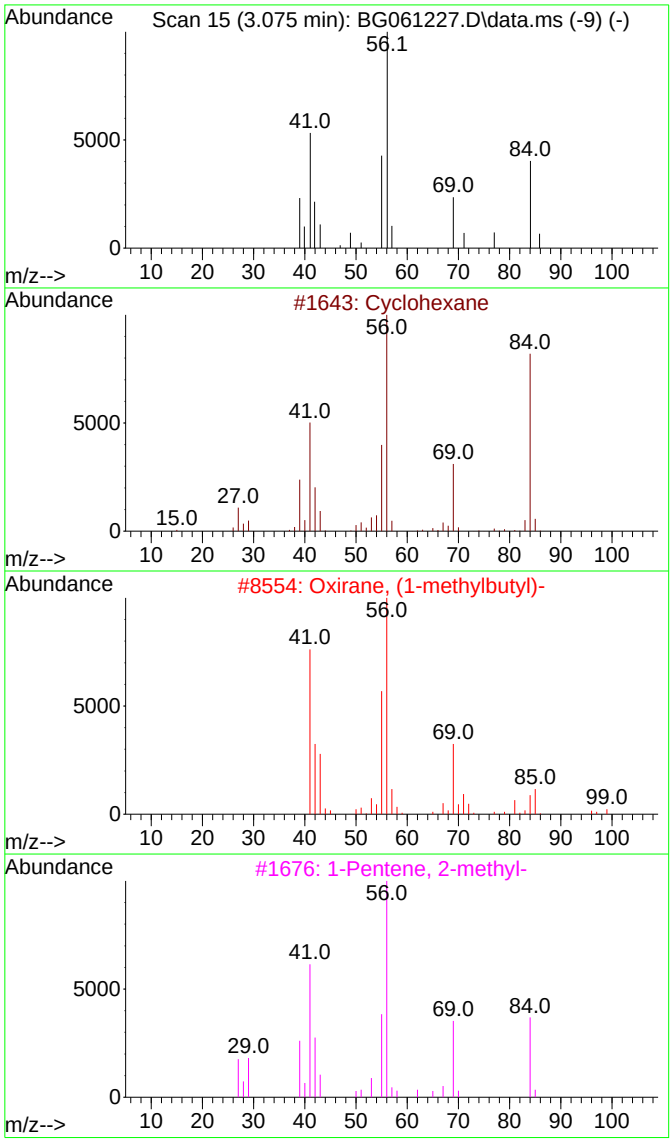
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

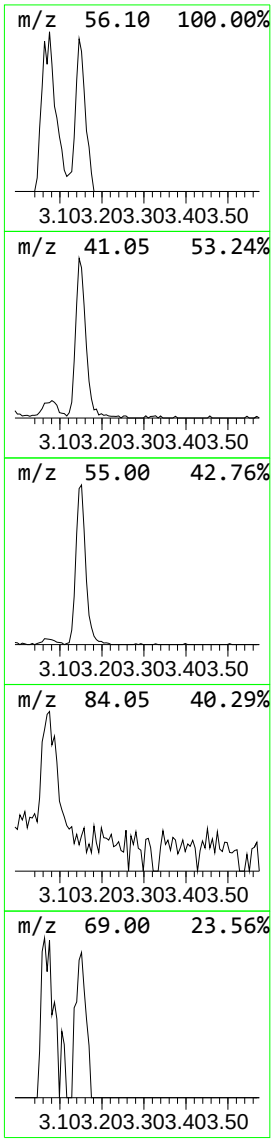
****

Peak Number 1 Cyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.075	2.38 ng	20592	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	72
2	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	42
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	36
4	Pentane, 3-methylene-	84	C6H12	000760-21-4	16
5	3-Buten-1-ol, 3-methyl-	86	C5H10O	000763-32-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061227.D
Acq On : 16 May 2024 19:23
Operator : MA/JU
Sample : P2480-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-MH-JJ

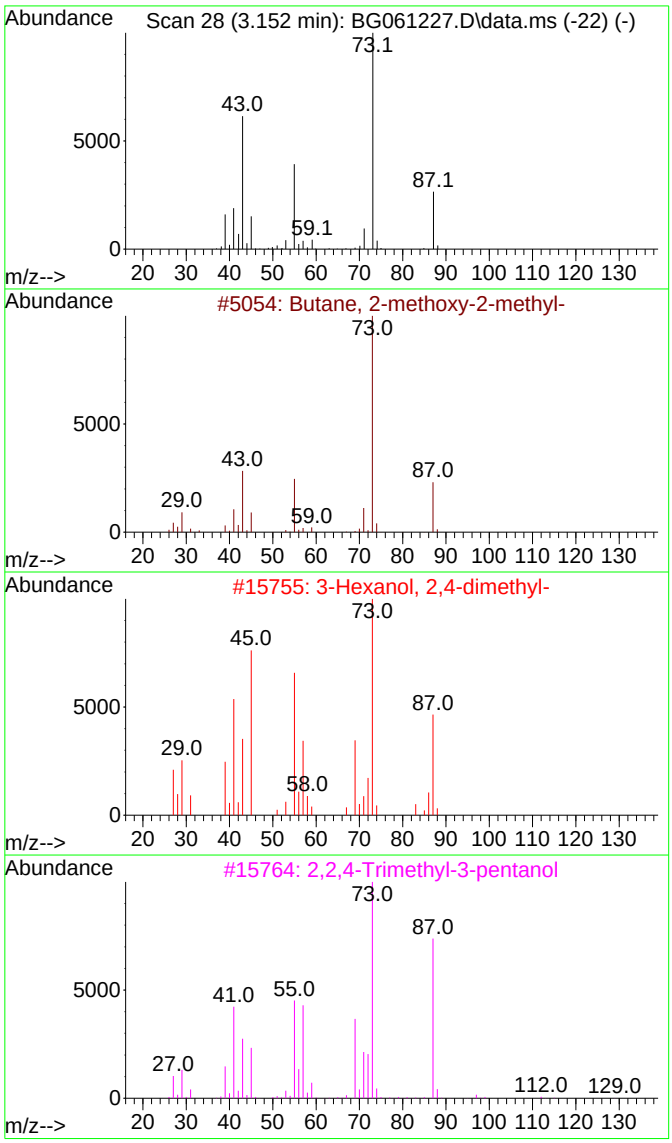
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

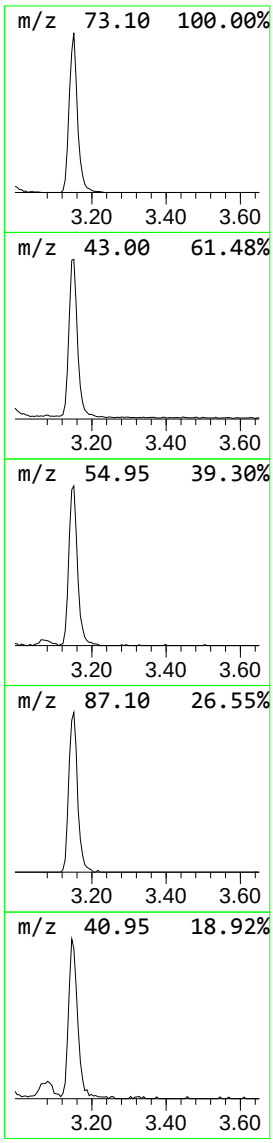
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	46.66 ng	404373	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	38
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061227.D
Acq On : 16 May 2024 19:23
Operator : MA/JU
Sample : P2480-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-MH-JJ

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

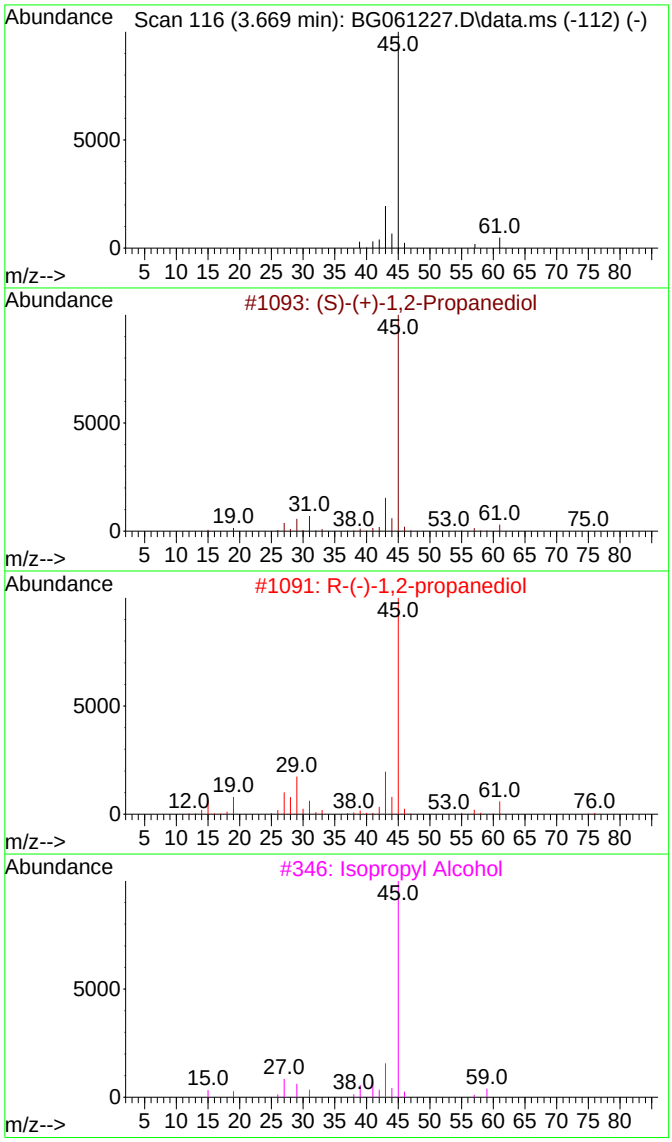
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

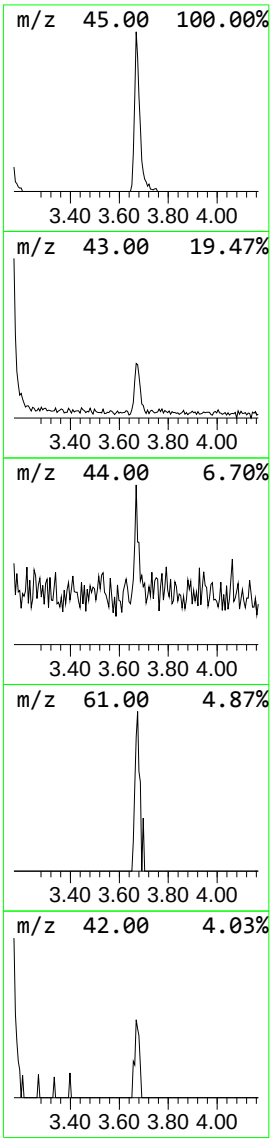
****

Peak Number 3 (S)-(+)-1,2-Propanediol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.669	3.83 ng	33202	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	Formamide	45	CH3NO	000075-12-7	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061227.D
Acq On : 16 May 2024 19:23
Operator : MA/JU
Sample : P2480-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-MH-JJ

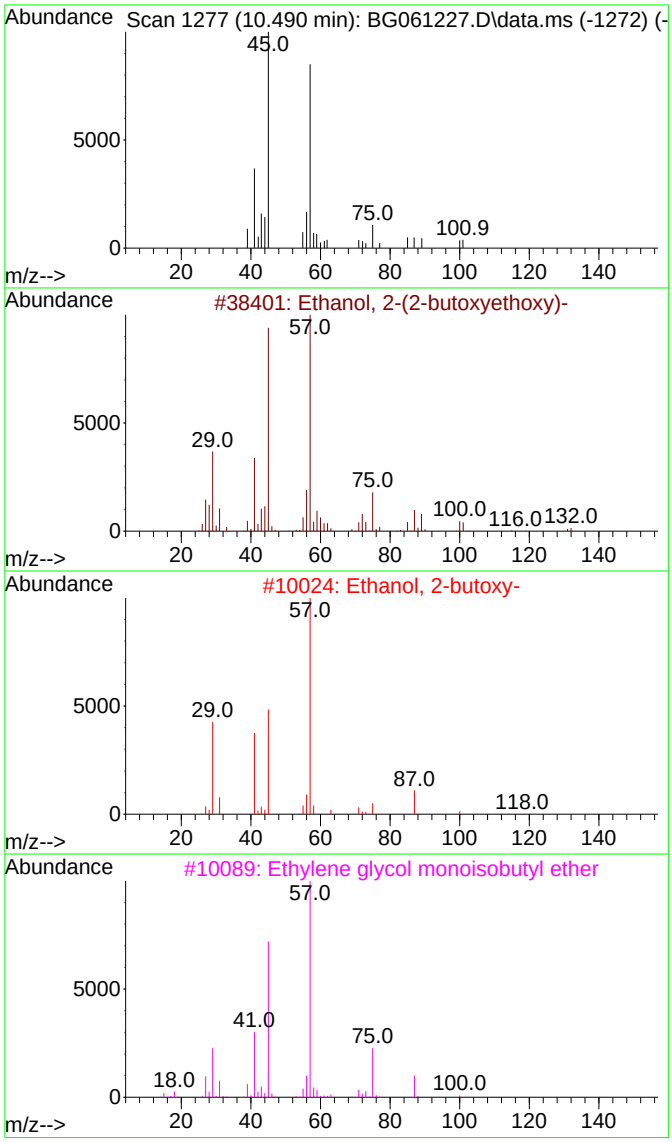
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

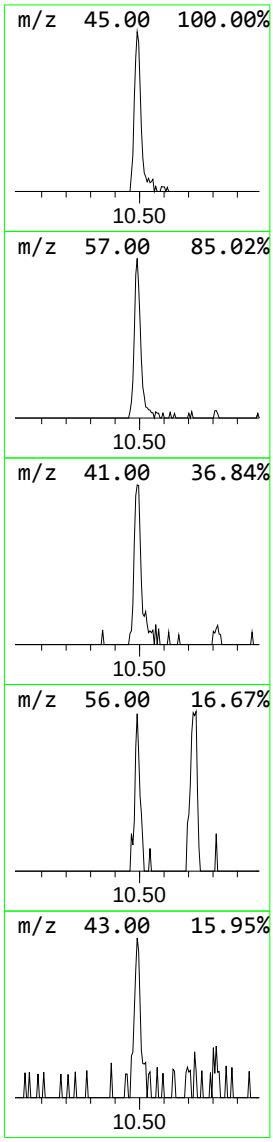
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.490	3.40 ng	41115	Naphthalene-d8	10.719

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
2	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	42
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061227.D
Acq On : 16 May 2024 19:23
Operator : MA/JU
Sample : P2480-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-MH-JJ

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

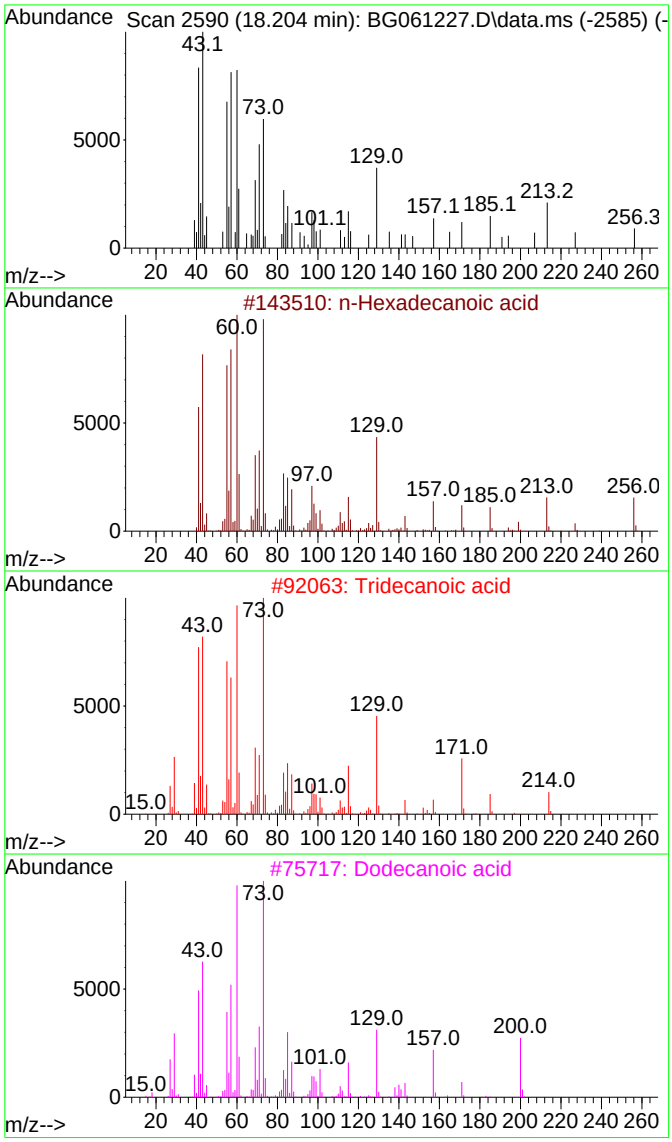
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

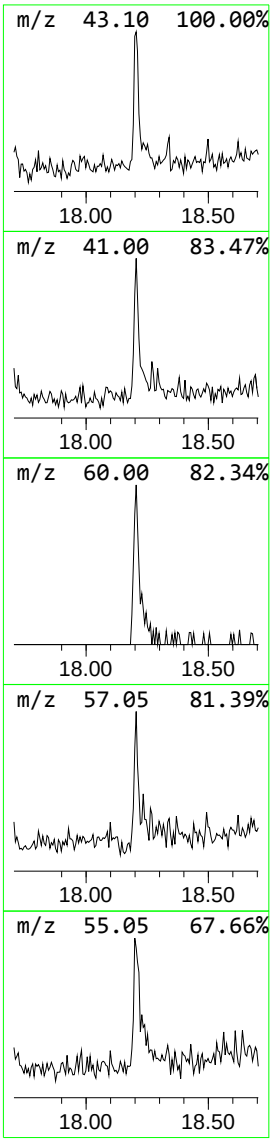
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.204	2.36 ng	53409	Phenanthrene-d10	17.305

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	50
3	Dodecanoic acid	200	C12H24O2	000143-07-7	47
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061227.D
Acq On : 16 May 2024 19:23
Operator : MA/JU
Sample : P2480-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-MH-JJ

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

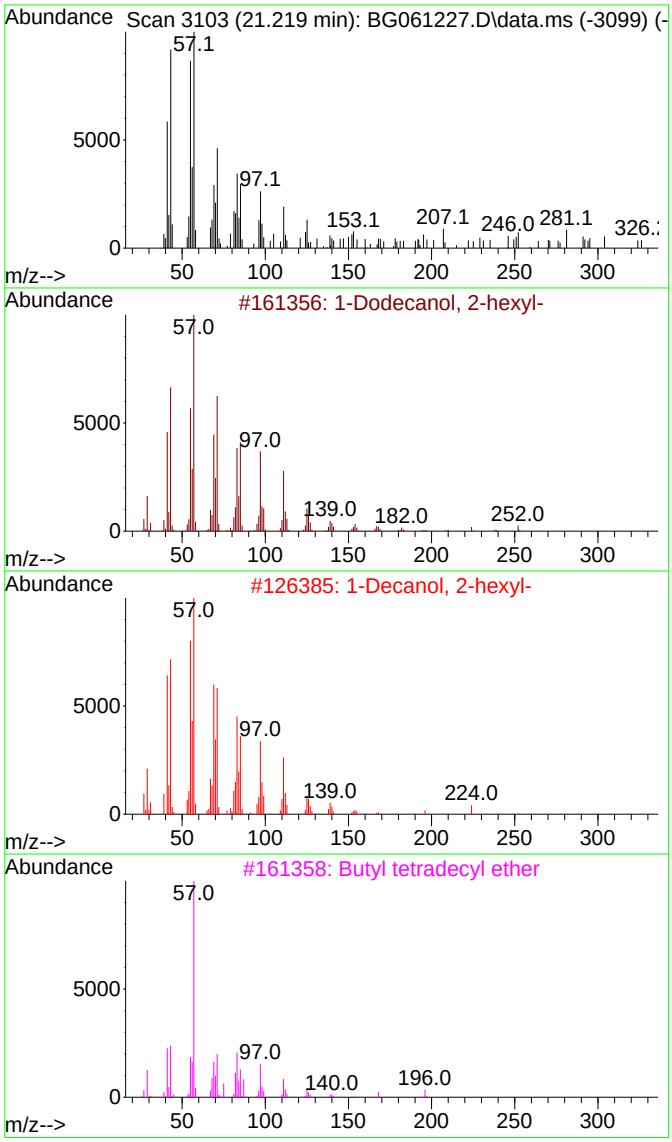
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

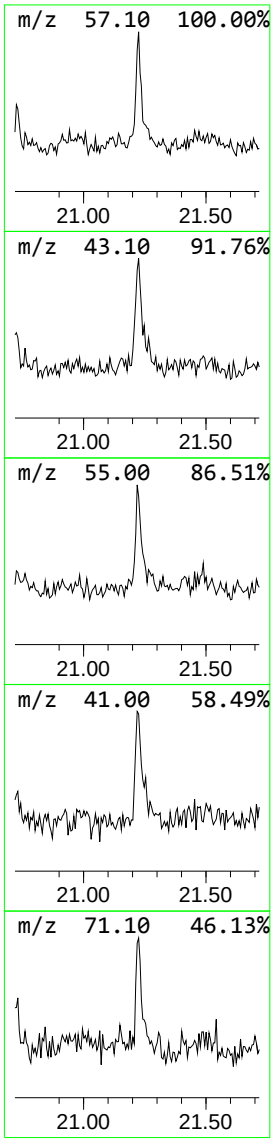
****

Peak Number 6 1-Dodecanol, 2-hexyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.219	3.44 ng	85203	Chrysene-d12	21.559

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	68
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	68
3	Butyl tetradecyl ether	270	C18H38O	1000406-40-4	68
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	64
5	Benzene, 1-(dodecyloxy)-2-nitro-	307	C18H29NO3	083027-71-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061227.D
Acq On : 16 May 2024 19:23
Operator : MA/JU
Sample : P2480-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-MH-JJ

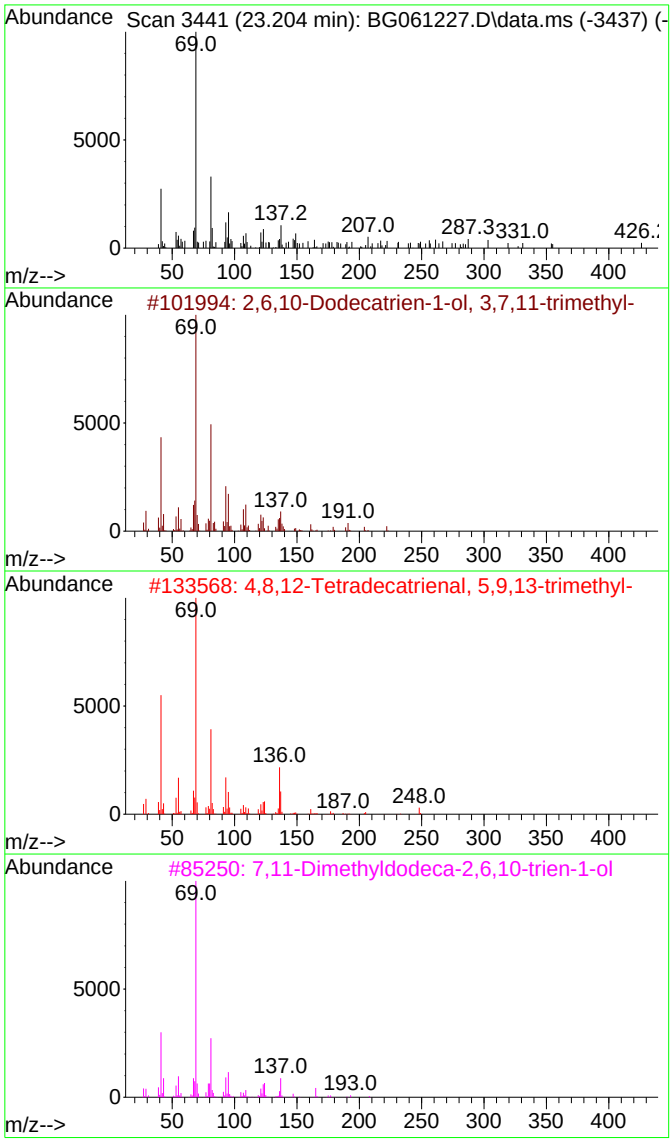
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

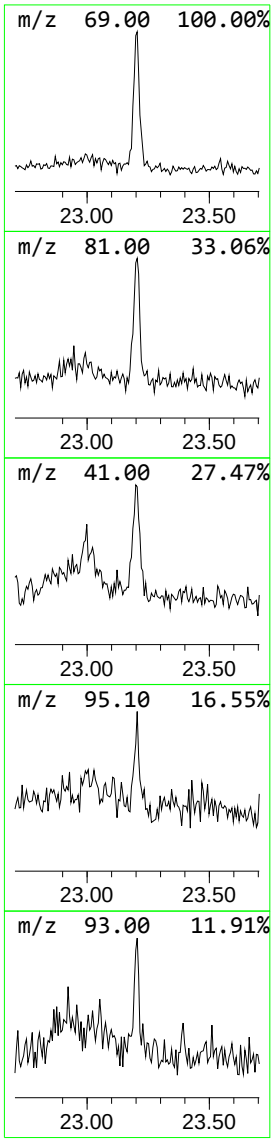
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.204	2.17 ng	60404	Perylene-d12	24.679

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	68
2	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	59
5	1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061227.D
Acq On : 16 May 2024 19:23
Operator : MA/JU
Sample : P2480-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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
Cyclohexane	3.075	2.4	ng	20592	1	7.928	173340	20.0
Butane, 2-metho...	3.152	46.7	ng	404373	1	7.928	173340	20.0
(S)-(+)-1,2-Pro...	3.669	3.8	ng	33202	1	7.928	173340	20.0
Ethanol, 2-(2-b...	10.490	3.4	ng	41115	2	10.719	241995	20.0
n-Hexadecanoic ...	18.204	2.4	ng	53409	4	17.305	452101	20.0
1-Dodecanol, 2-...	21.219	3.4	ng	85203	5	21.559	495414	20.0
2,6,10-Dodecatr...	23.204	2.2	ng	60404	6	24.679	556595	20.0