LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021577.D
Acq On : 20 Aug 2024 18:07
Operator : RC/JU
Sample : P3643-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
924-K1-SD-0.5-1.0-081524

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_P\Methods\8270E-BP081324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP021577.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	25	rVB	4000161	4805839	38.24%	6.415%
2	3.546	91	95	108	rVB	122822	178509	1.42%	0.238%
3	4.940	326	332	340	rVB	211667	311300	2.48%	0.416%
4	5.399	403	410	421	rBV	4042616	5900412	46.95%	7.875%
5	6.969	668	677	687	rBV	3930906	6152705	48.95%	8.212%
6	7.804	811	819	826	rBV	1064340	1711426	13.62%	2.284%
7	8.951	1005	1014	1023	rBV	2225100	3779747	30.07%	5.045%
8	9.516	1103	1110	1116	rBV	101317	157752	1.26%	0.211%
9	10.593	1285	1293	1302	rBV	1310457	2331284	18.55%	3.112%
10	11.334	1411	1419	1430	rBV2	212882	383326	3.05%	0.512%
11	13.063	1704	1713	1724	rBV	4824039	7442551	59.22%	9.934%
12	14.451	1940	1949	1960	rBV	2044091	3223262	25.65%	4.302%
13	14.686	1979	1989	2002	rBV	1386776	3122148	24.84%	4.167%
14	15.969	2199	2207	2217	rBV	4328196	6686619	53.20%	8.925%
15	17.263	2420	2427	2437	rBV	2560238	4071911	32.40%	5.435%
16	18.216	2583	2589	2598	rBV	294941	505955	4.03%	0.675%
17	19.533	2809	2813	2822	rBV2	111033	171727	1.37%	0.229%
18	19.986	2884	2890	2896	rBV	10108373	12568287	100.00%	16.775%
19	21.398	3126	3130	3137	rBV	609809	919016	7.31%	1.227%
20	21.727	3179	3186	3195	rBV	3299643	5008659	39.85%	6.685%
21	25.168	3762	3771	3784	rVB	1938944	5488922	43.67%	7.326%

Sum of corrected areas: 74921357

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021577.D
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Misc :
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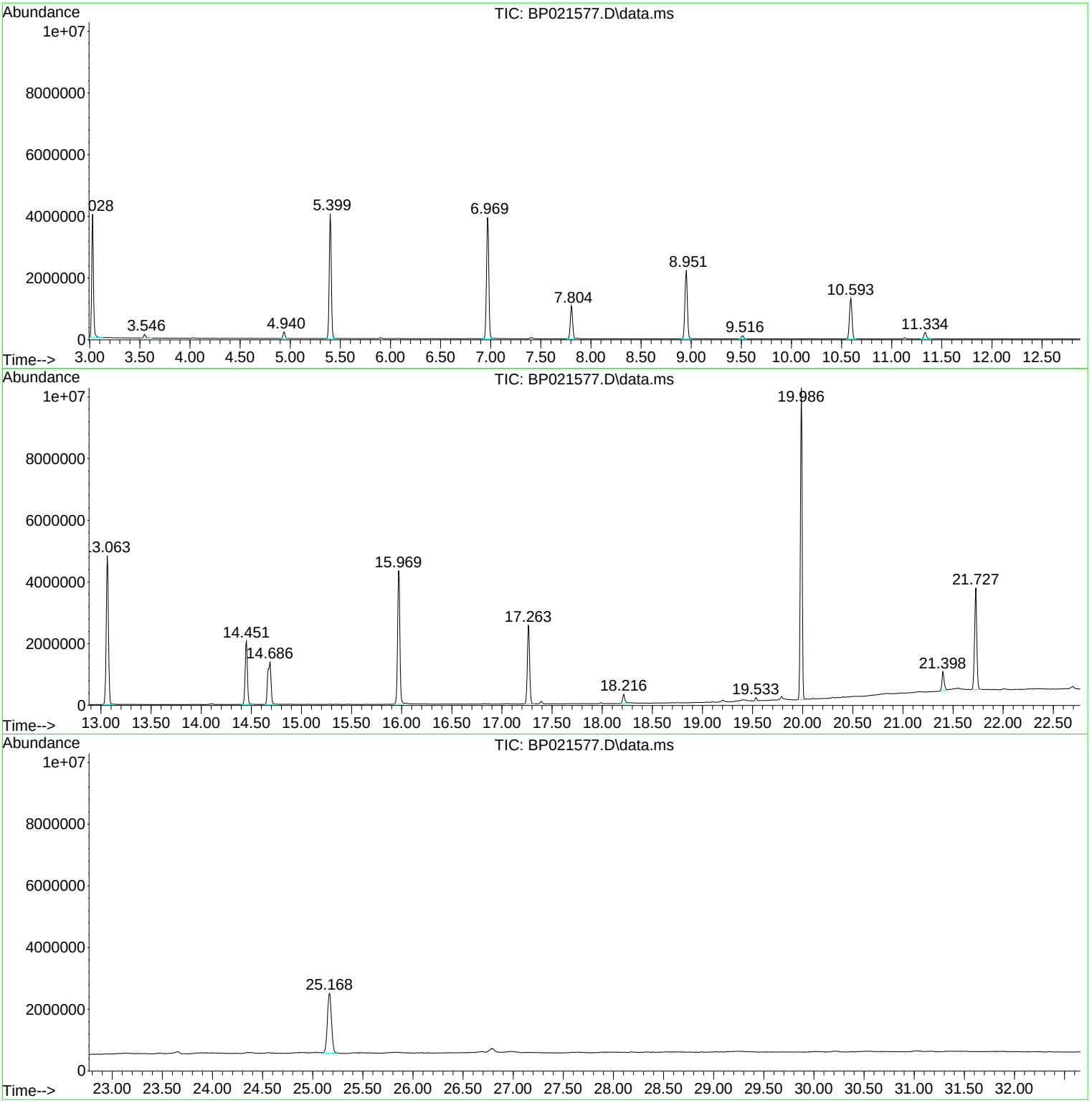
Instrument :
BNA_P
ClientSampleId :
924-K1-SD-0.5-1.0-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.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_P\Data\BP082024\
Data File : BP021577.D
Acq On : 20 Aug 2024 18:07
Operator : RC/JU
Sample : P3643-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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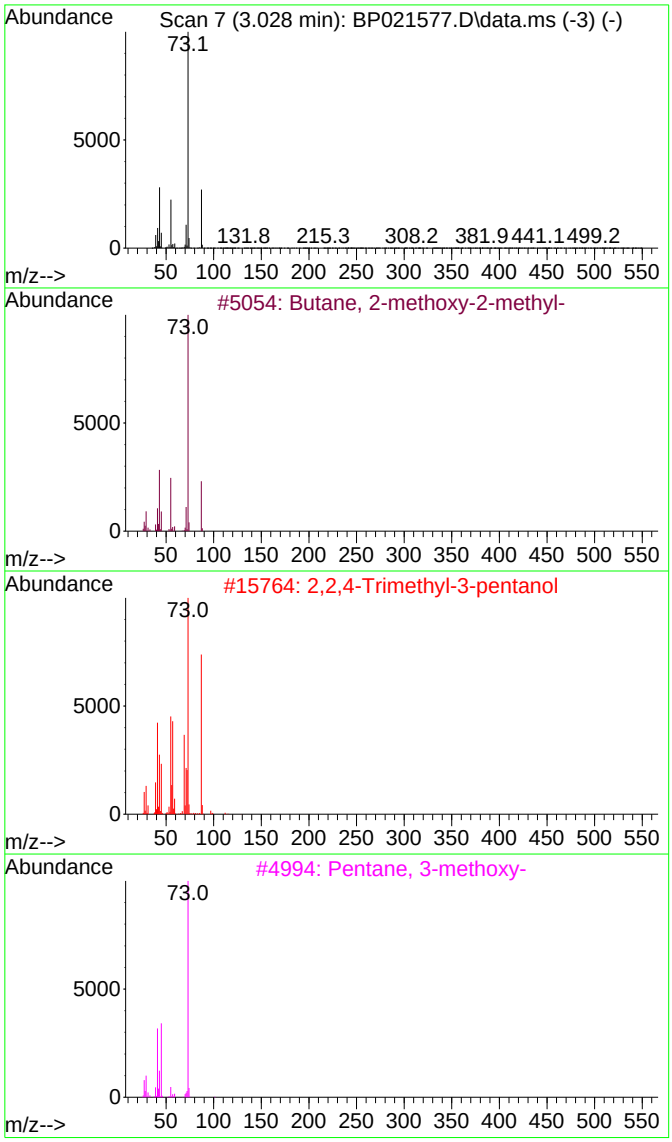
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

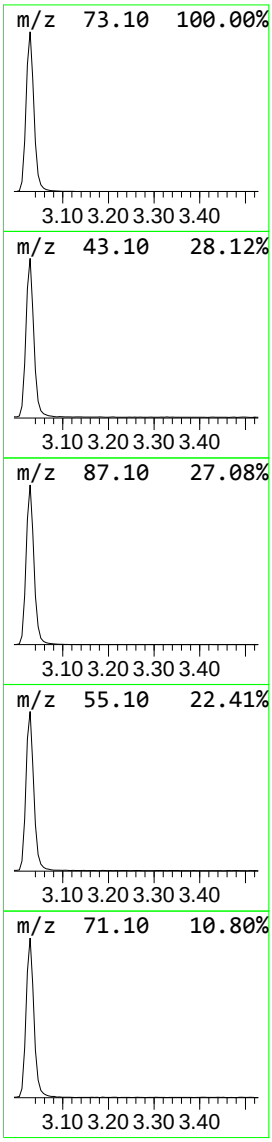
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	56.16 ng	4805840	1,4-Dichlorobenzene-d4	7.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021577.D
Acq On : 20 Aug 2024 18:07
Operator : RC/JU
Sample : P3643-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
924-K1-SD-0.5-1.0-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

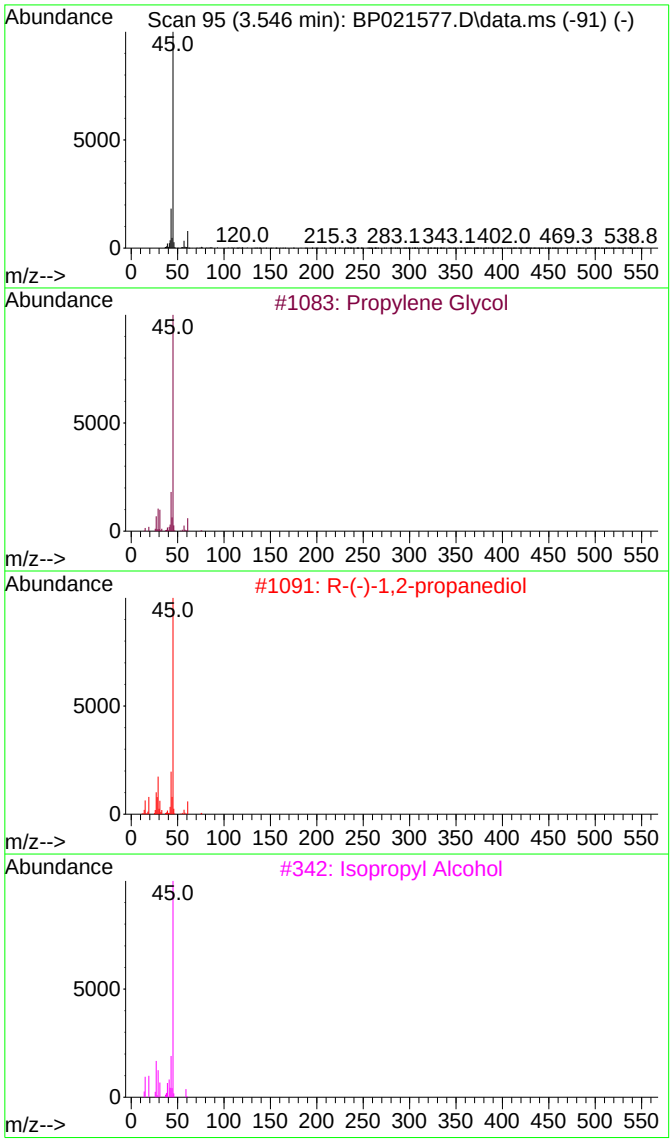
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

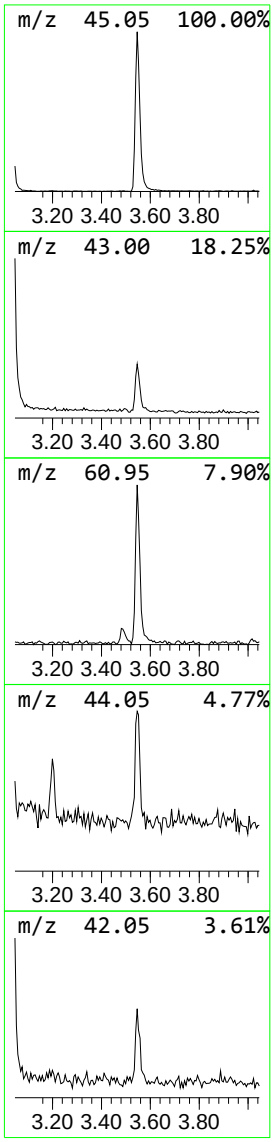
****

Peak Number 2 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.546	2.09 ng	178509	1,4-Dichlorobenzene-d4	7.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021577.D
Acq On : 20 Aug 2024 18:07
Operator : RC/JU
Sample : P3643-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
924-K1-SD-0.5-1.0-081524

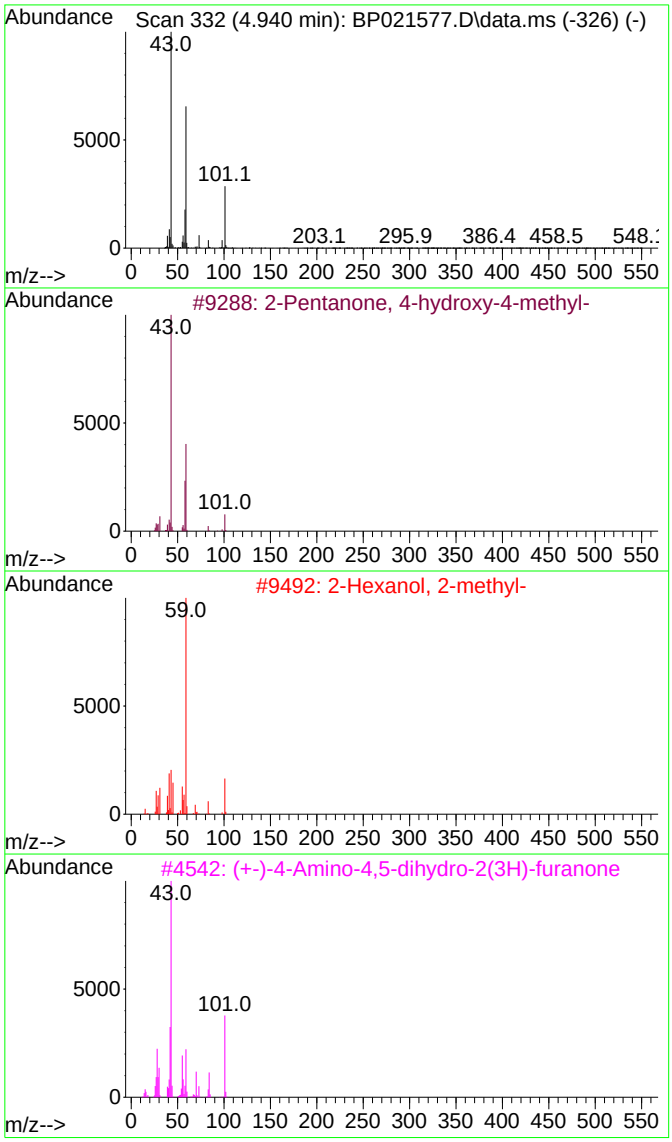
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

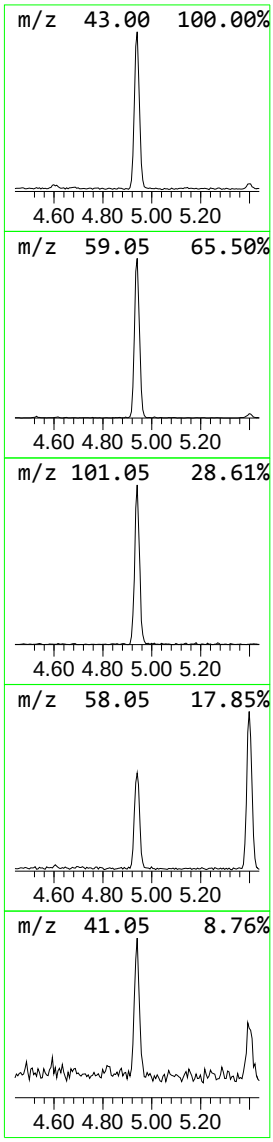
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	3.64 ng	311300	1,4-Dichlorobenzene-d4	7.804

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	50
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	40
5	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021577.D
Acq On : 20 Aug 2024 18:07
Operator : RC/JU
Sample : P3643-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
924-K1-SD-0.5-1.0-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

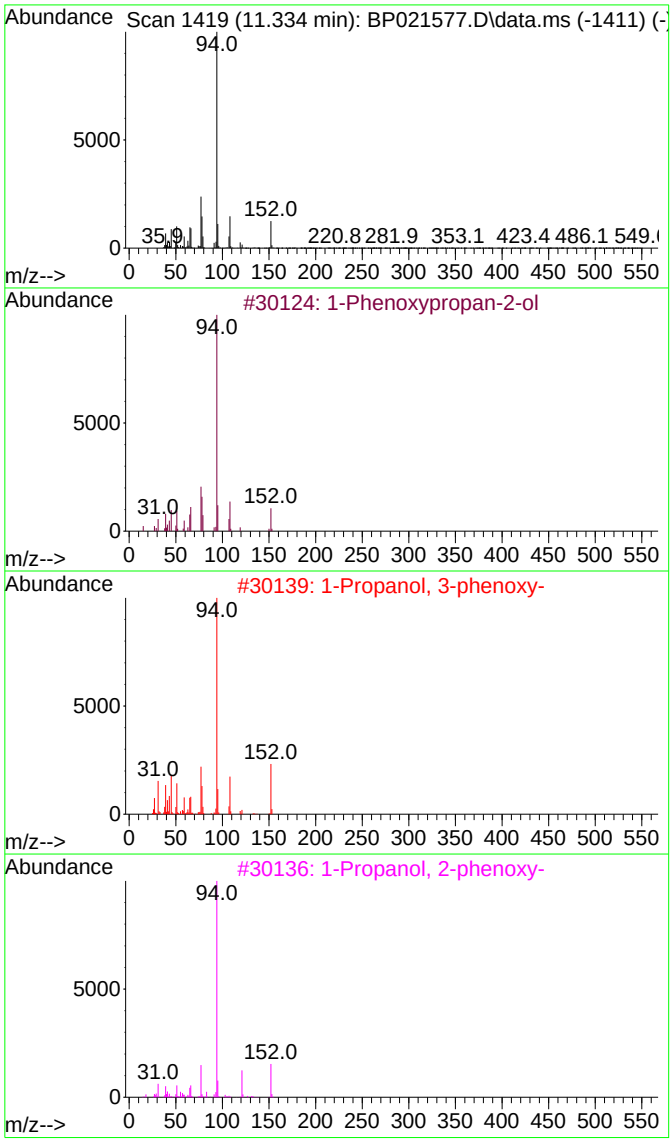
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

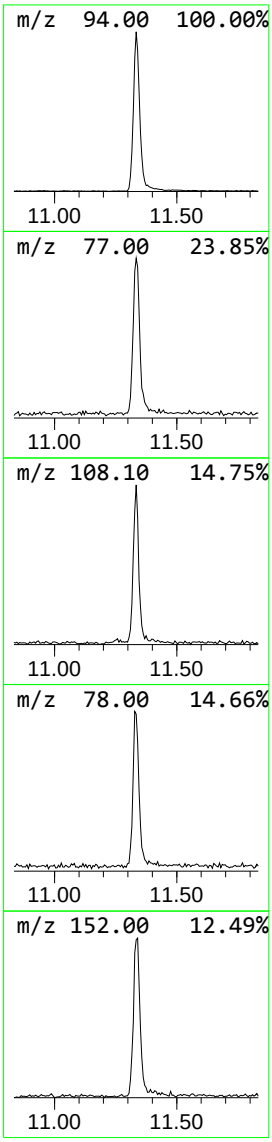
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.334	3.29 ng	383326	Naphthalene-d8	10.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	72
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	Carbonic acid, sec-butyl phenyl ...	194	C11H14O3	013183-17-0	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021577.D
Acq On : 20 Aug 2024 18:07
Operator : RC/JU
Sample : P3643-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
924-K1-SD-0.5-1.0-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

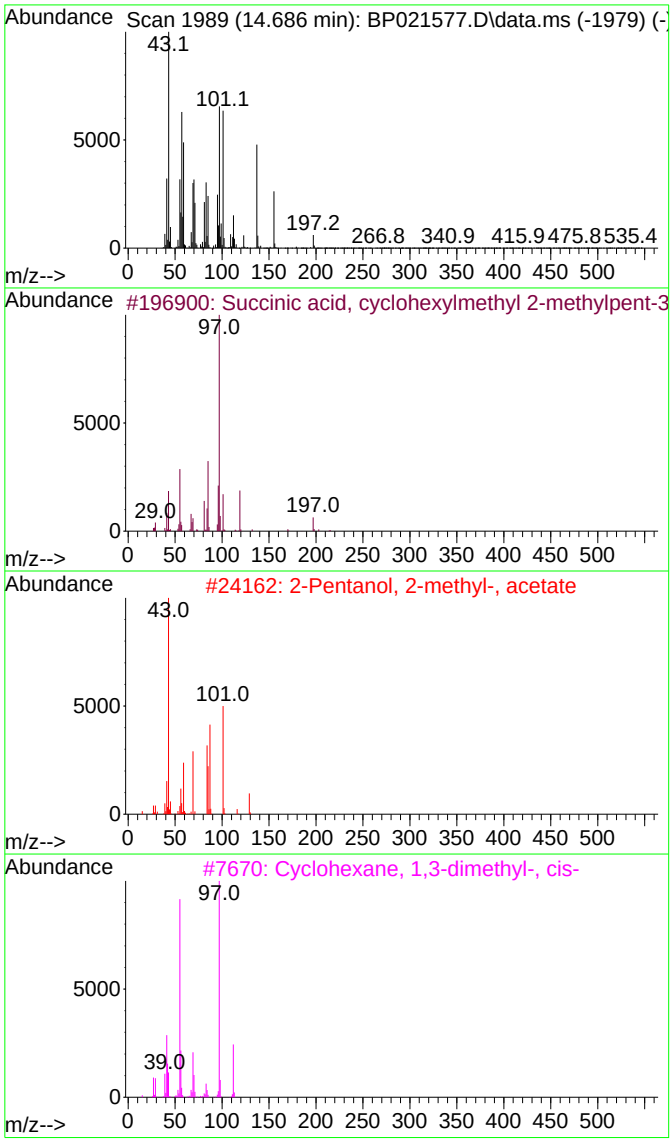
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

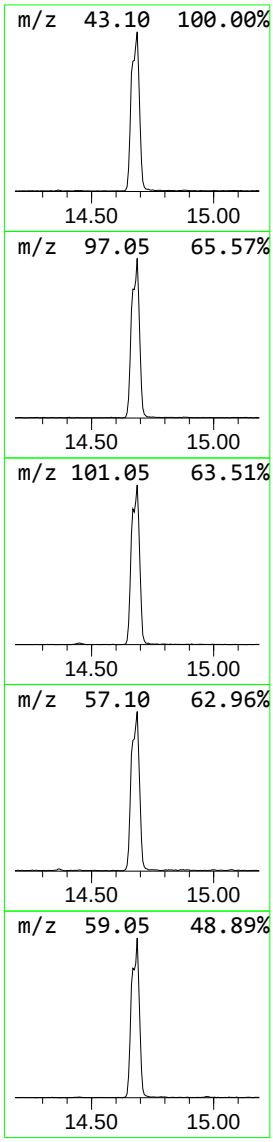
****

Peak Number 5 unknown14.687 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.687	19.37 ng	3122150	Acenaphthene-d10	14.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, cyclohexylmethyl ...	298	C17H30O4	1000389-60-0	14
2	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	14
3	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	11
4	Cyclohexane, 1,3-dimethyl-	112	C8H16	000591-21-9	11
5	1-(2-Furyl)-3-buten-1-ol	138	C8H10O2	1000311-94-9	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
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Sample : P3643-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
924-K1-SD-0.5-1.0-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

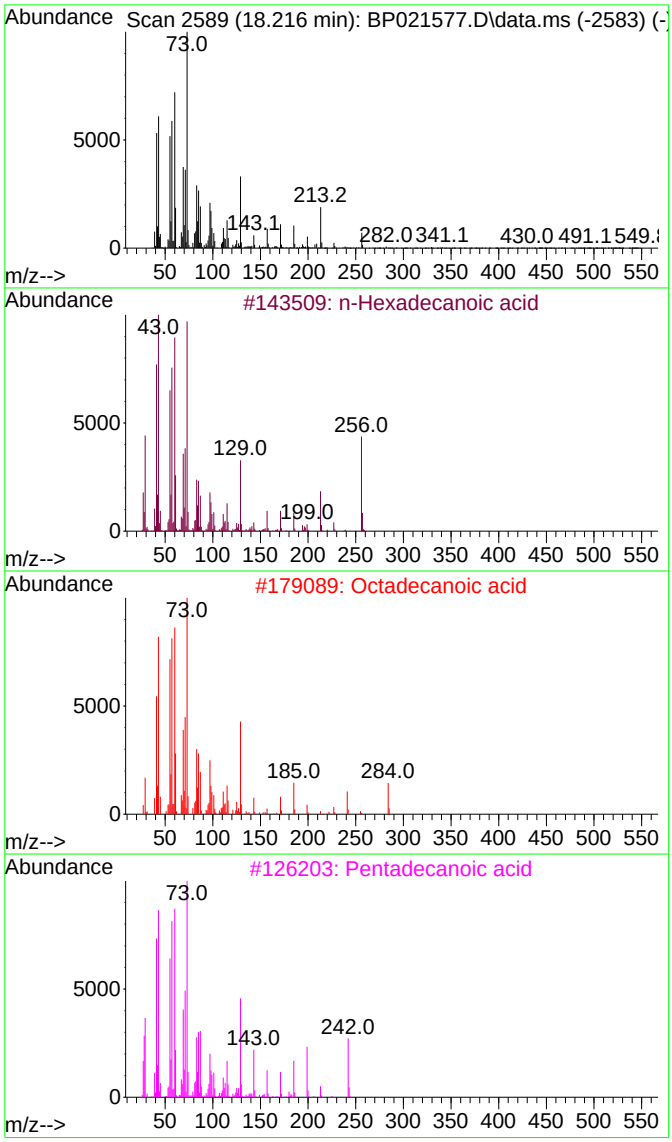
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

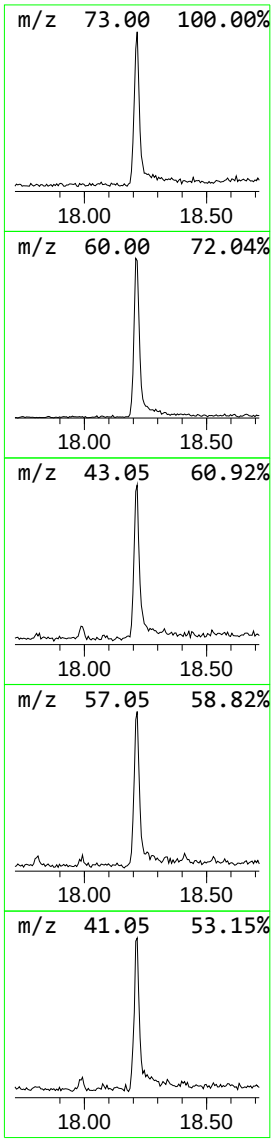
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	2.49 ng	505955	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Ether, dodecyl isopropyl	228	C15H32O	029379-42-8	25





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Sample : P3643-10
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
924-K1-SD-0.5-1.0-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

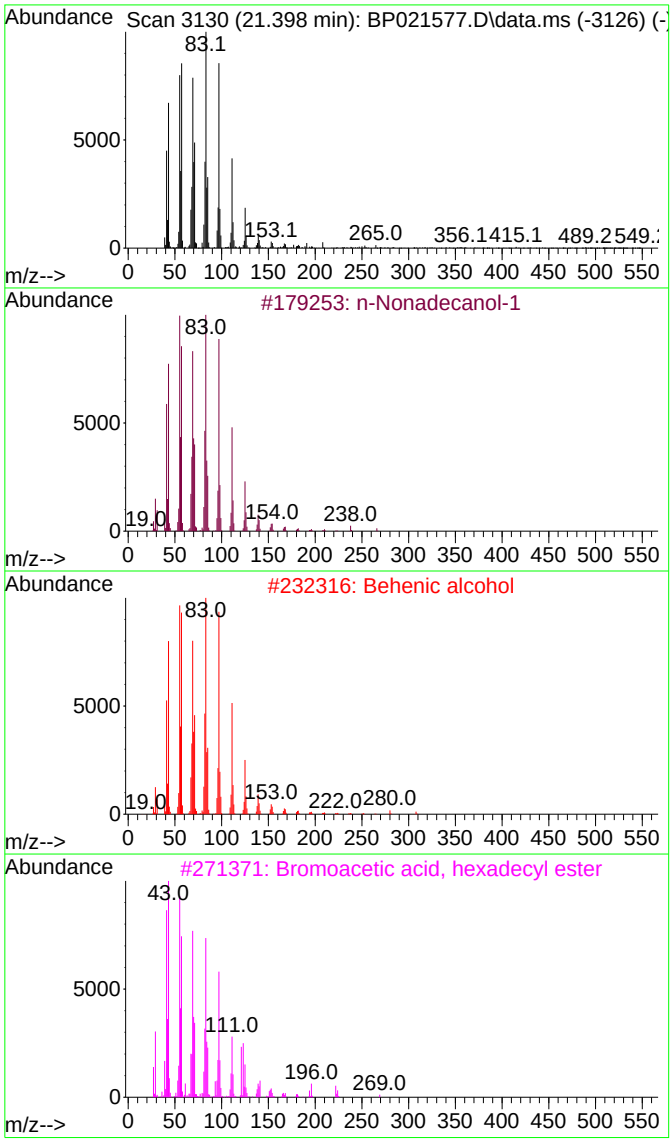
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

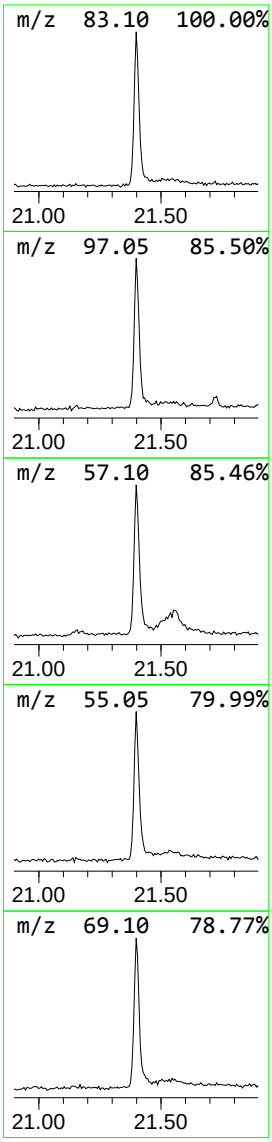
****

Peak Number 7 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.398	3.67 ng	919016	Chrysene-d12	21.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
5	1-Tetracosene	336	C24H48	010192-32-2	91





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.028	56.2	ng	4805840	1	7.804	1711430	20.0
Propylene Glycol	3.546	2.1	ng	178509	1	7.804	1711430	20.0
2-Pentanone, 4-...	4.940	3.6	ng	311300	1	7.804	1711430	20.0
1-Phenoxypropan...	11.334	3.3	ng	383326	2	10.592	2331280	20.0
unknown14.687	14.687	19.4	ng	3122150	3	14.451	3223260	20.0
n-Hexadecanoic ...	18.216	2.5	ng	505955	4	17.263	4071910	20.0
n-Nonadecanol-1	21.398	3.7	ng	919016	5	21.727	5008660	20.0