LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060724\
Data File : BP020563.D
Acq On : 07 Jun 2024 16:59
Operator : MA/JU
Sample : P2715-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPM

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-BP052924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP020563.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	37	rVB	2478690	3941316	21.47%	3.543%
2	3.558	92	97	113	rVB	852859	1162170	6.33%	1.045%
3	5.375	399	406	423	rBV	6450796	9714674	52.93%	8.732%
4	6.934	659	671	690	rBV	6040442	9882145	53.84%	8.883%
5	7.357	737	743	755	rBV	298593	466876	2.54%	0.420%
6	7.752	802	810	817	rBV	1383567	2180399	11.88%	1.960%
7	8.904	996	1006	1016	rBV	3856012	6491456	35.37%	5.835%
8	9.457	1094	1100	1110	rVB	223748	336453	1.83%	0.302%
9	10.528	1273	1282	1292	rBV	1843877	2986070	16.27%	2.684%
10	11.263	1399	1407	1421	rBV	612318	1109069	6.04%	0.997%
11	12.992	1693	1701	1720	rBV	8713868	13534889	73.75%	12.166%
12	14.381	1929	1937	1945	rBV	2564578	3845960	20.96%	3.457%
13	14.616	1975	1977	1992	rVB	6683512	7584713	41.33%	6.818%
14	15.904	2188	2196	2206	rBV	7045818	11063572	60.28%	9.945%
15	17.198	2409	2416	2421	rBV	3082475	4355983	23.73%	3.916%
16	18.151	2571	2578	2586	rBV	1146199	1926295	10.50%	1.732%
17	19.327	2775	2778	2784	rBV	81708	184562	1.01%	0.166%
18	19.480	2799	2804	2811	rBV	489788	761891	4.15%	0.685%
19	19.927	2874	2880	2891	rBV	13619181	18353062	100.00%	16.497%
20	21.339	3115	3120	3126	rBV	874012	1482080	8.08%	1.332%
21	21.657	3167	3174	3181	rBV	2687322	4627967	25.22%	4.160%
22	25.015	3736	3745	3756	rVB	1831143	5257977	28.65%	4.726%

Sum of corrected areas: 111249579

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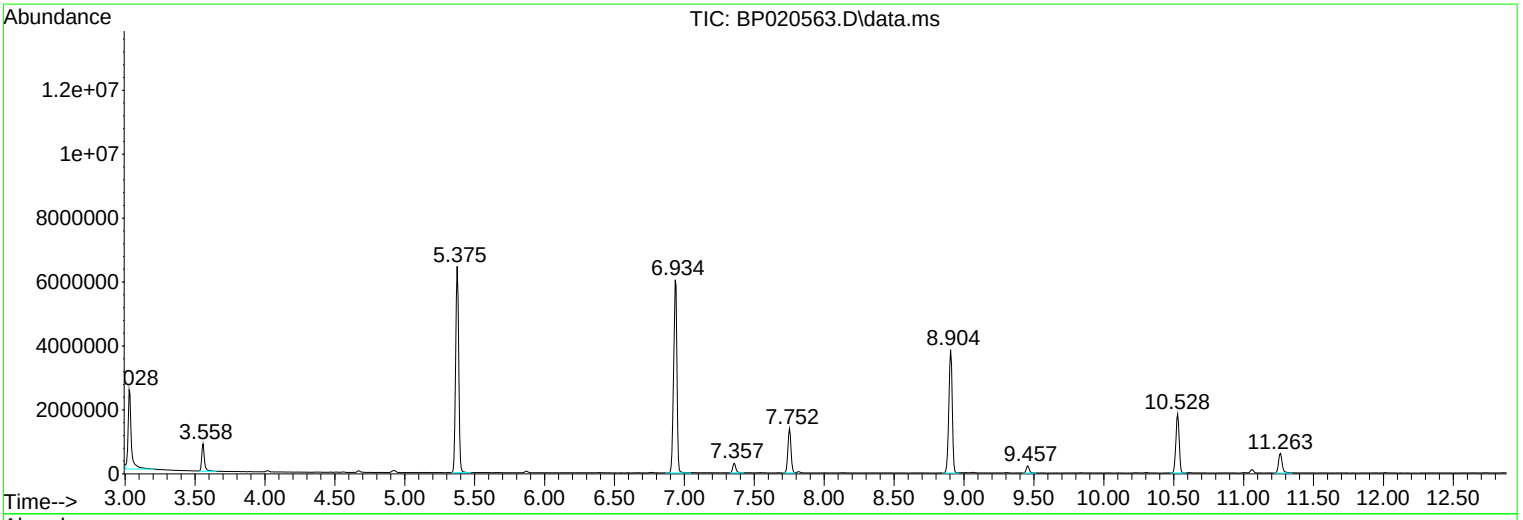
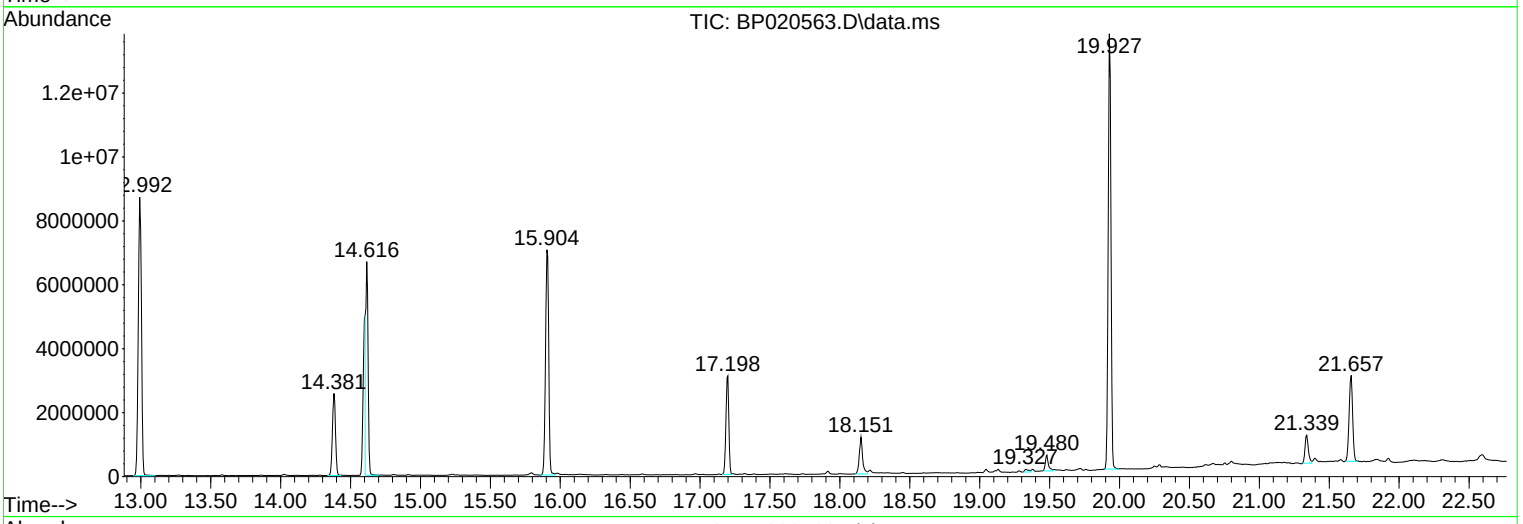
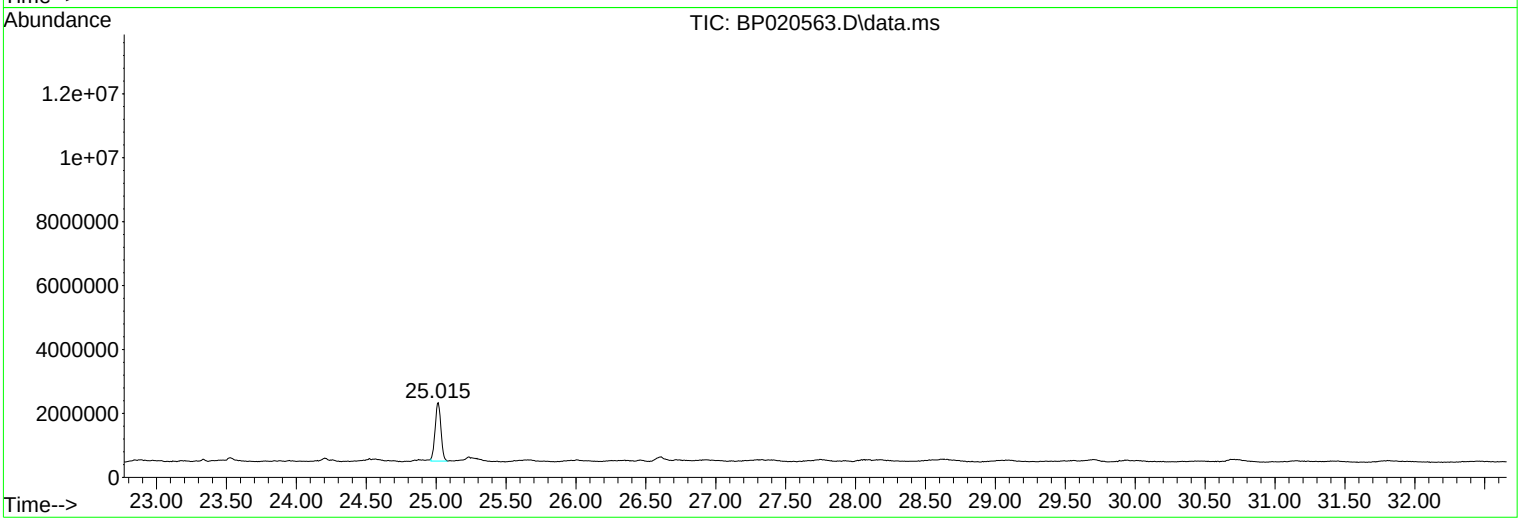
ClientSampleId :
WCS-TPM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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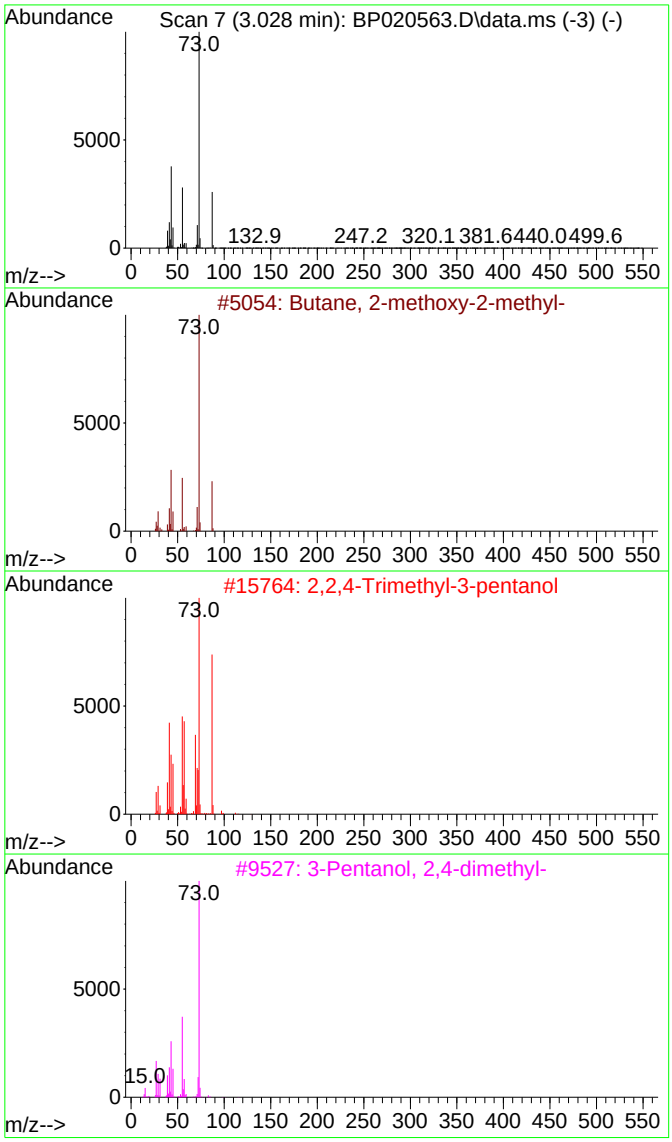
TIC Integration Parameters: LSCINT.P

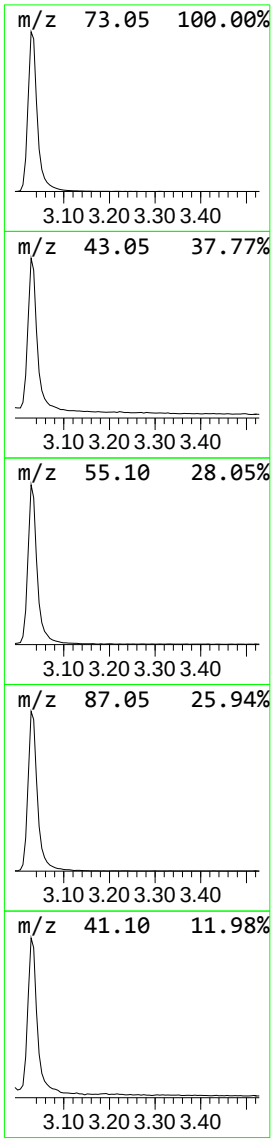
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	36.15 ng	3941320	1,4-Dichlorobenzene-d4	7.752

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22





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Data File : BP020563.D
Acq On : 07 Jun 2024 16:59
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Sample : P2715-05
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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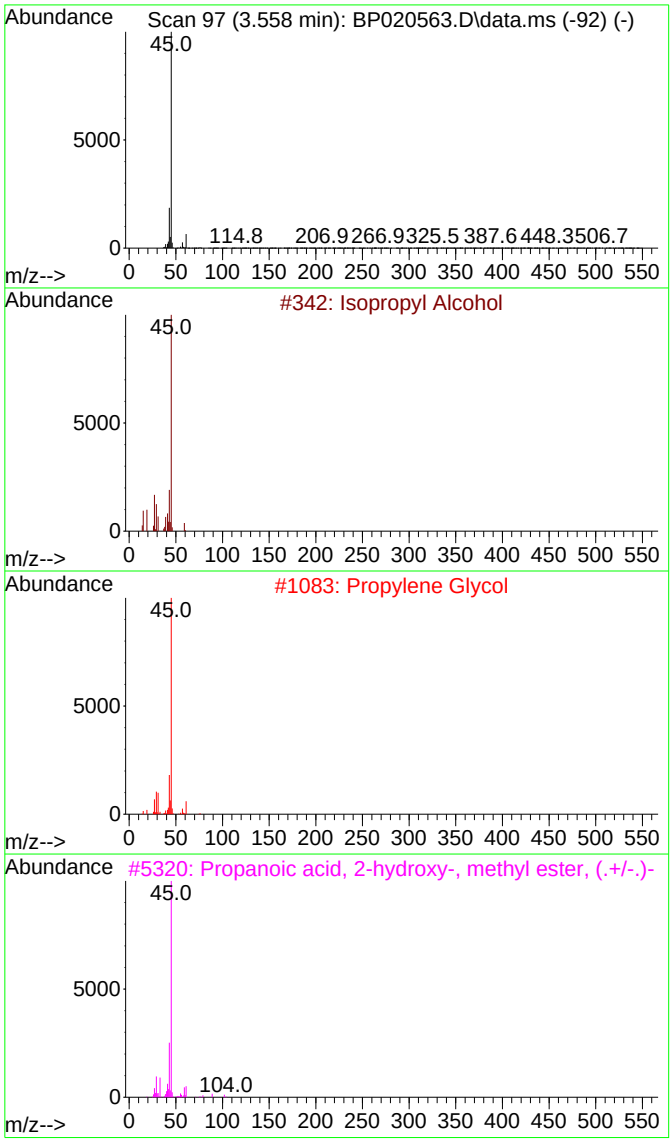
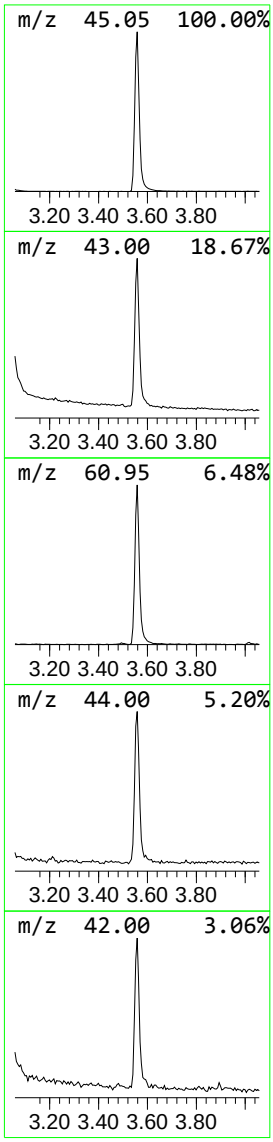
Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.558	10.66 ng	1162170	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2	Propylene Glycol	76	C3H8O2	000057-55-6	47
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9





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Data File : BP020563.D
Acq On : 07 Jun 2024 16:59
Operator : MA/JU
Sample : P2715-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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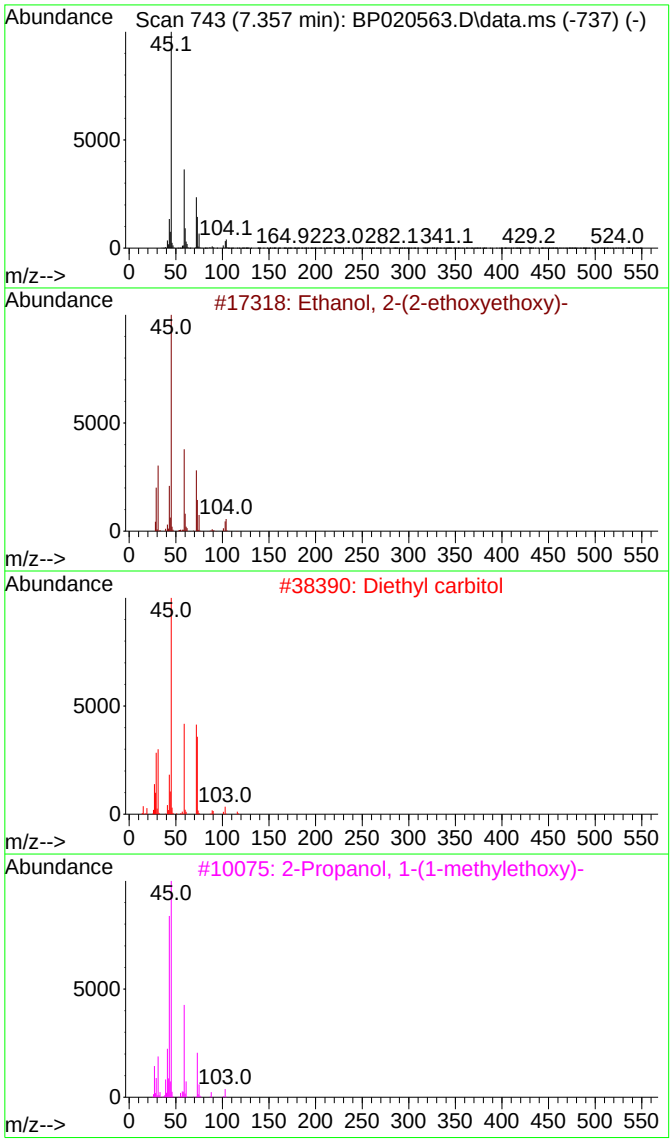
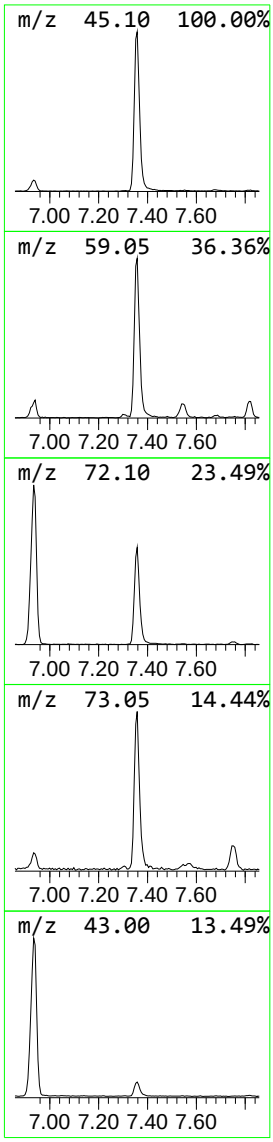
****
Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.357	4.28 ng	466876	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	40





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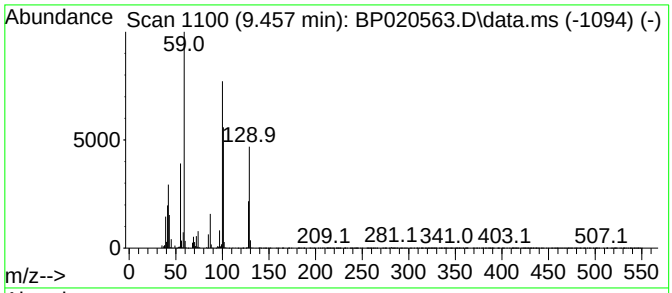
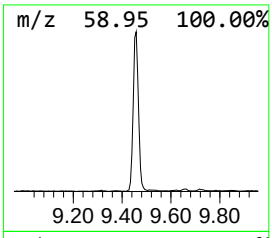
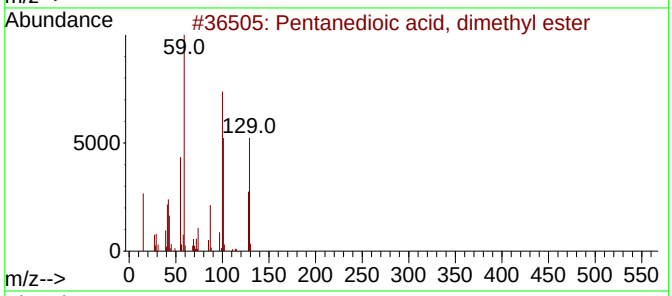
****
Peak Number 4 Pentanedioic acid, dimethyl... Concentration Rank 9

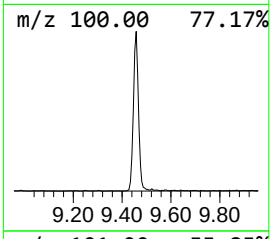
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.457	2.25 ng	336453	Naphthalene-d8	10.528

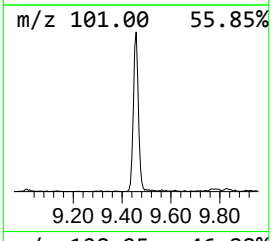
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	50
3	Butyric acid, 3-bromo-, methyl e...	180	C5H9BrO2	021249-59-2	27
4	Butanoic acid, 4-iodo-, methyl e...	228	C5H9IO2	014273-85-9	17
5	Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	16

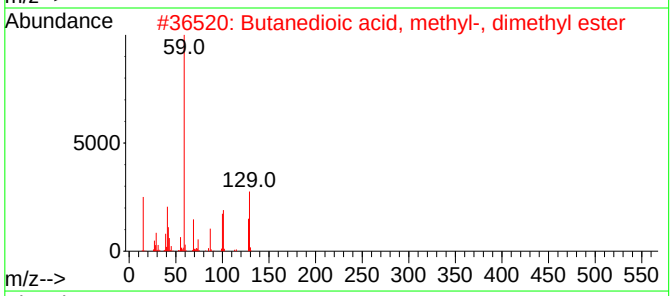


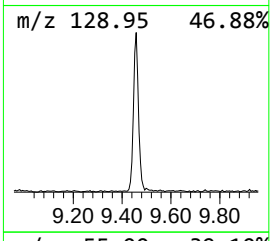


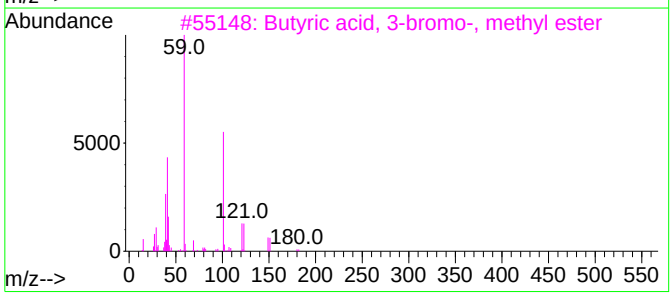


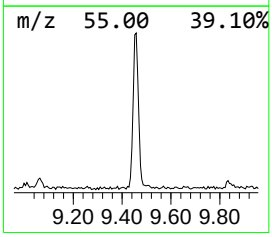












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

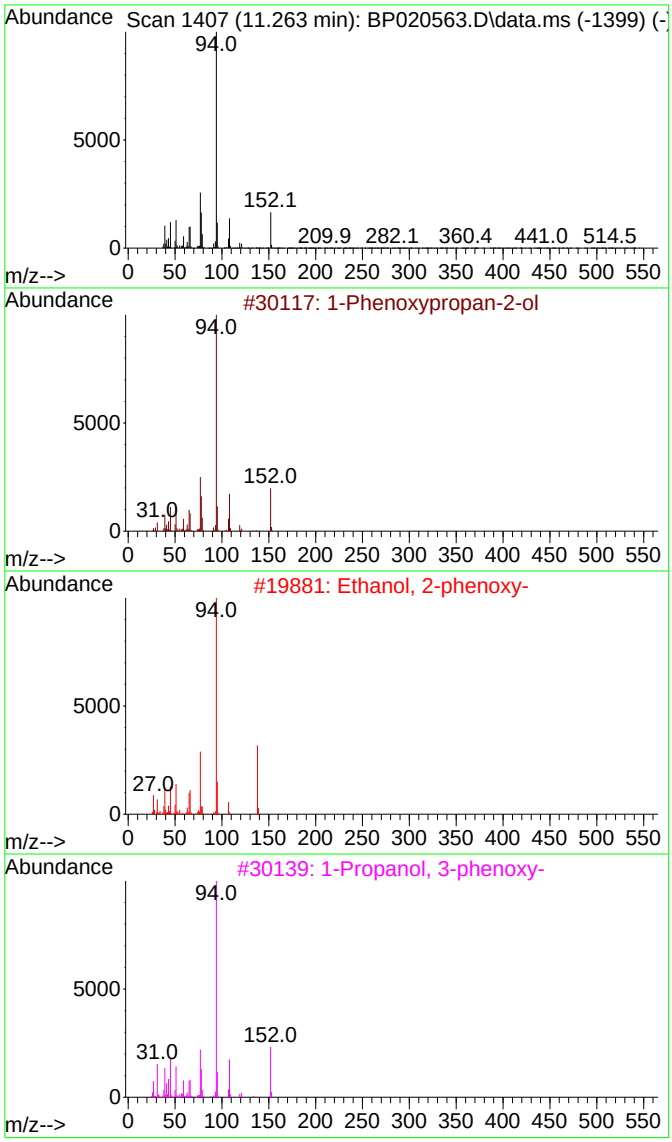
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

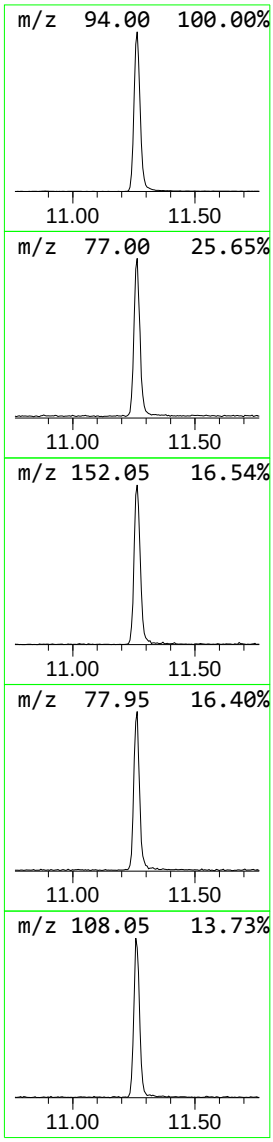
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.263	7.43 ng	1109070	Naphthalene-d8	10.528

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
3	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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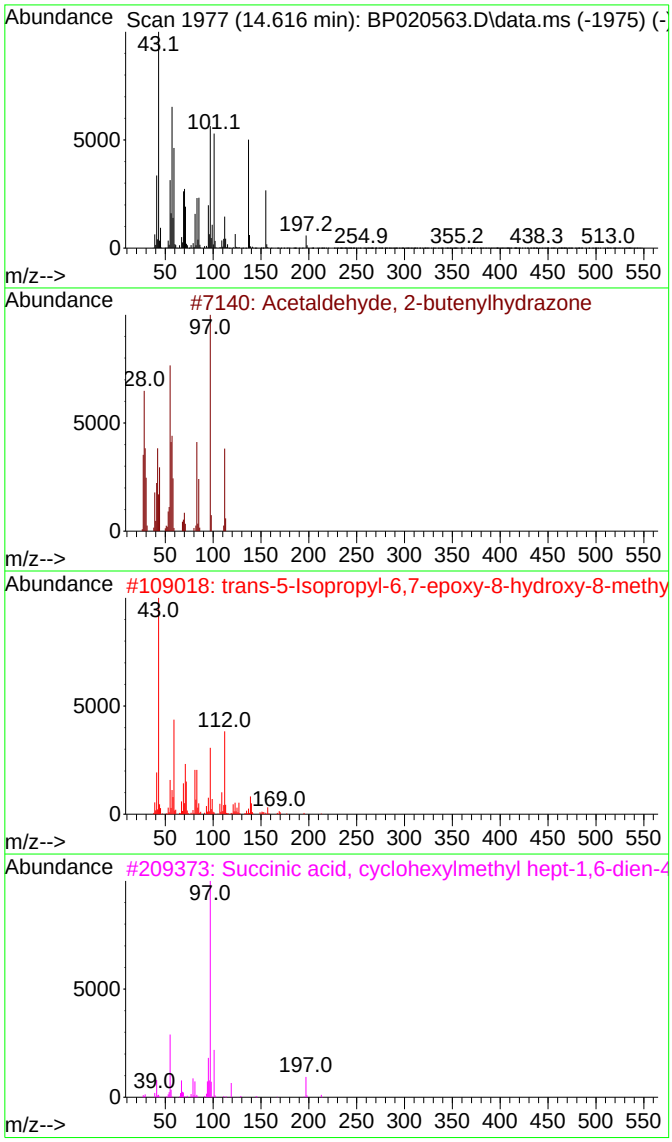
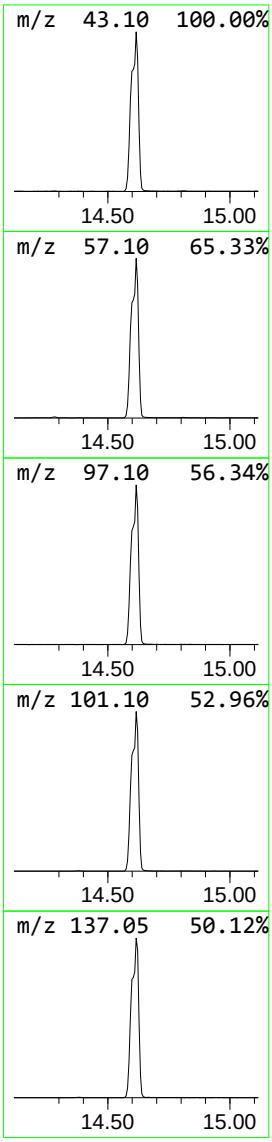
Peak Number 6 unknown14.616 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.616	39.44 ng	7584710	Acenaphthene-d10	14.381

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde, 2-butenylhydrazone	112	C6H12N2	075268-07-4	14
2	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
3	Succinic acid, cyclohexylmethyl ...	308	C18H28O4	1000391-33-3	10
4	Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	10
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10





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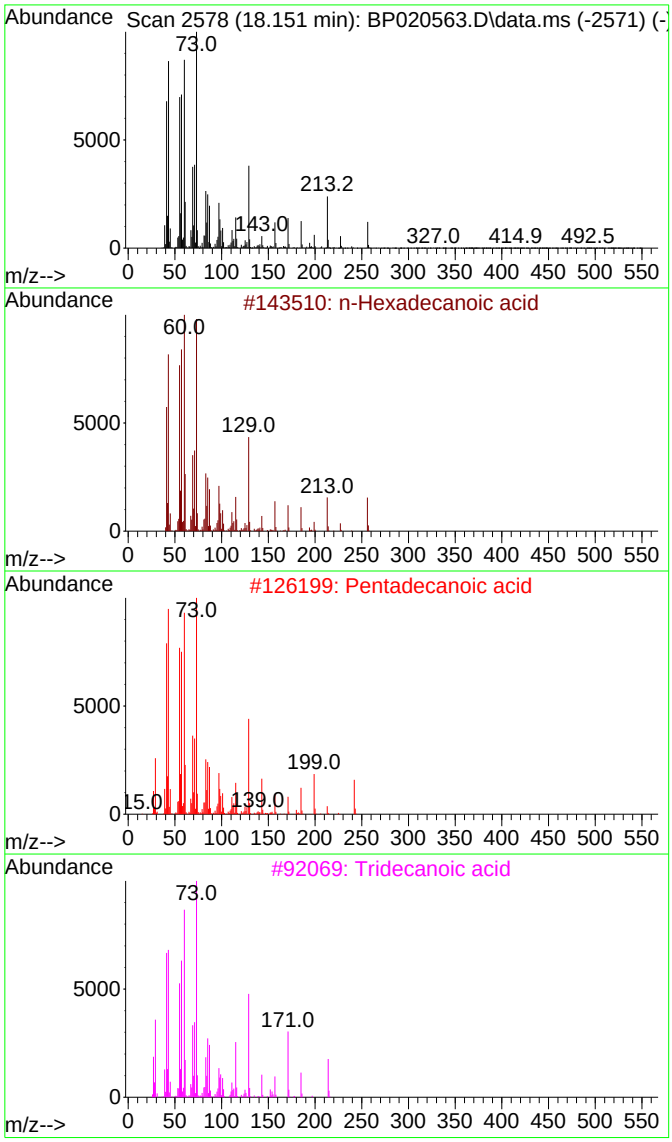
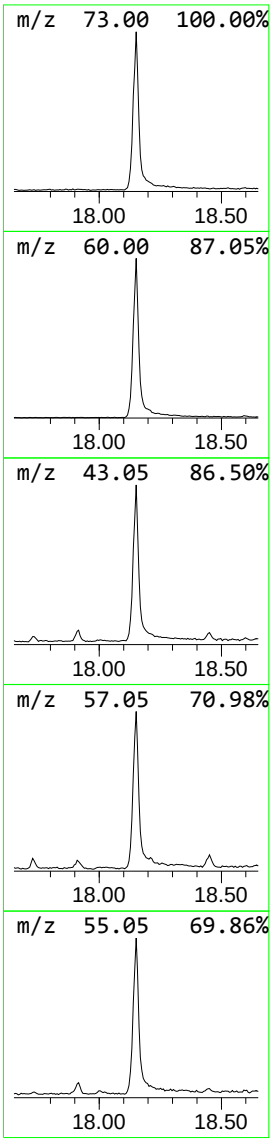
Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	8.84 ng	1926300	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
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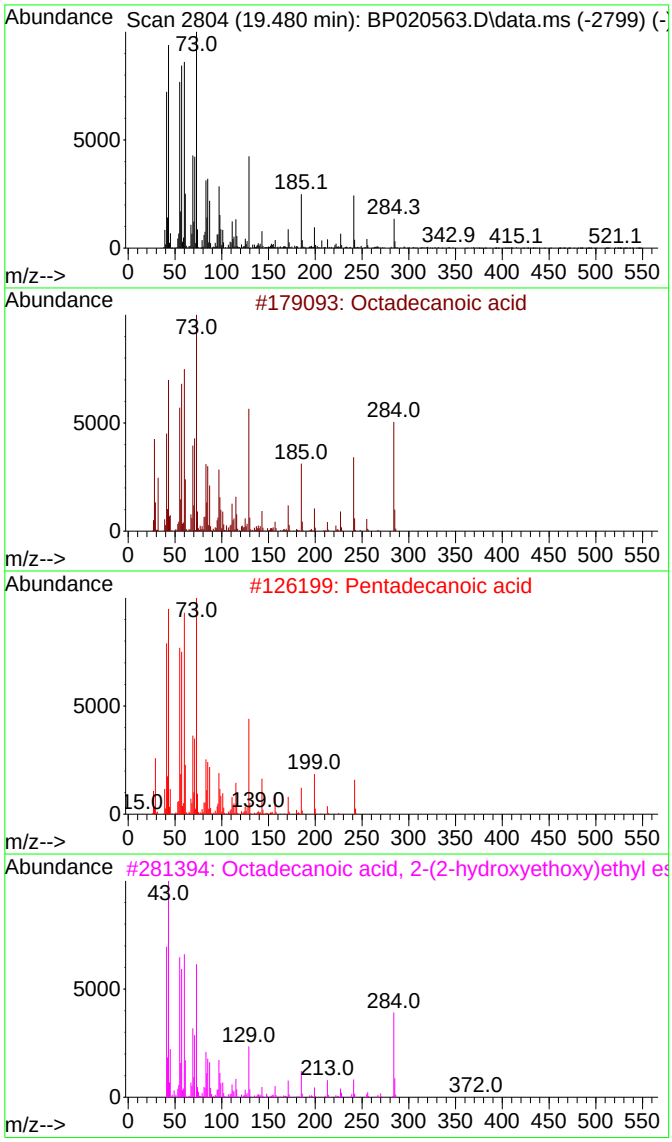
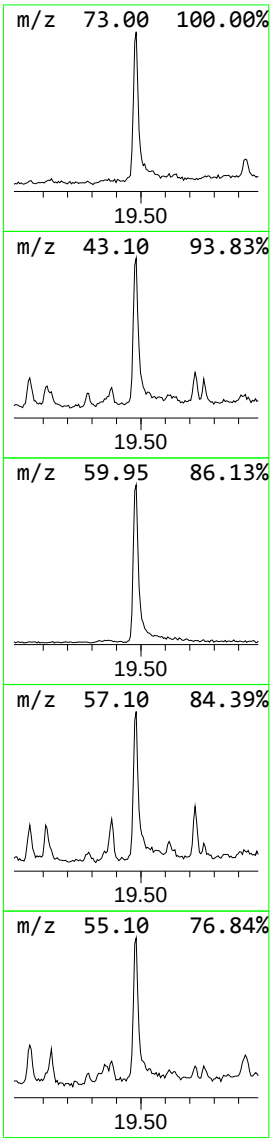
****

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.480	3.29 ng	761891	Chrysene-d12	21.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060724\
Data File : BP020563.D
Acq On : 07 Jun 2024 16:59
Operator : MA/JU
Sample : P2715-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPM

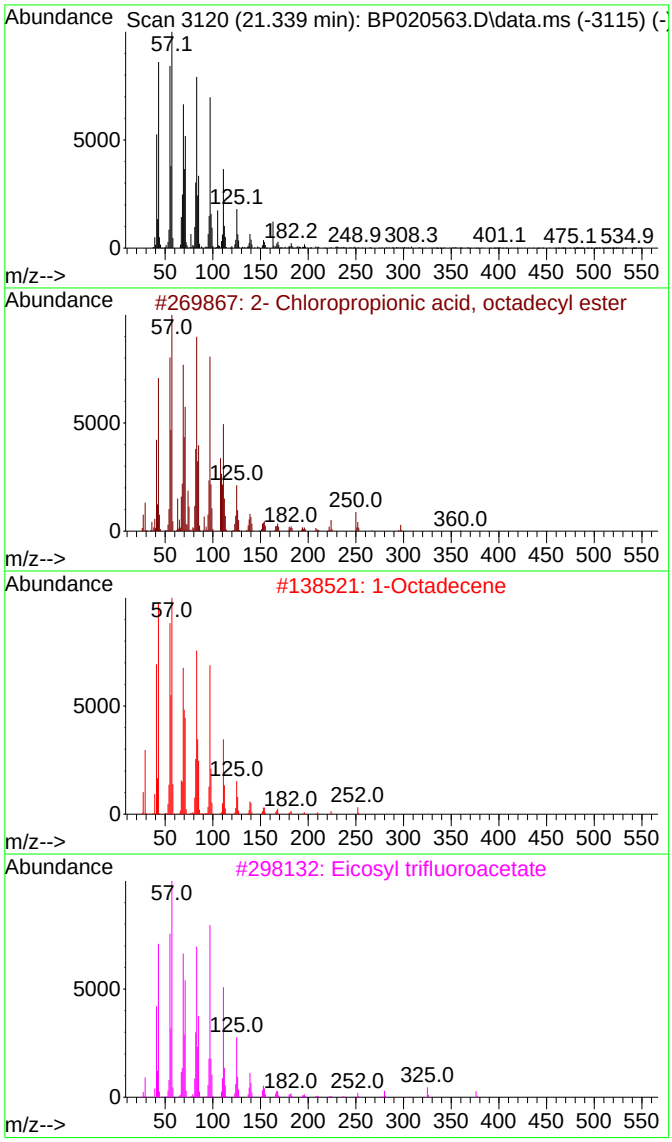
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

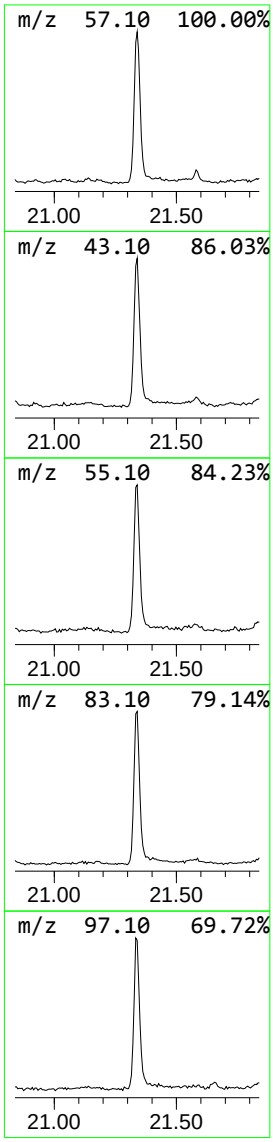
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2- Chloropropionic acid, oc... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.339	6.40 ng	1482080	Chrysene-d12	21.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	96
2	1-Octadecene	252	C18H36	000112-88-9	94
3	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	94
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	94
5	Behenic alcohol	326	C22H46O	000661-19-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060724\
Data File : BP020563.D
Acq On : 07 Jun 2024 16:59
Operator : MA/JU
Sample : P2715-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.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
Butane, 2-metho...	3.028	36.1	ng	3941320	1	7.752	2180400	20.0
Isopropyl Alcohol	3.558	10.7	ng	1162170	1	7.752	2180400	20.0
Ethanol, 2-(2-e...	7.357	4.3	ng	466876	1	7.752	2180400	20.0
Pentanedioic ac...	9.457	2.3	ng	336453	2	10.528	2986070	20.0
1-Phenoxypropan...	11.263	7.4	ng	1109070	2	10.528	2986070	20.0
unknown14.616	14.616	39.4	ng	7584710	3	14.381	3845960	20.0
n-Hexadecanoic ...	18.151	8.8	ng	1926300	4	17.198	4355980	20.0
Octadecanoic acid	19.480	3.3	ng	761891	5	21.657	4627970	20.0
2- Chloropropio...	21.339	6.4	ng	1482080	5	21.657	4627970	20.0