LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
Data File : BP020509.D
Acq On : 05 Jun 2024 00:06
Operator : MA/JU
Sample : P2689-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-05312024

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: BP020509.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.040	4	9	24	rVB	1959722	2998847	20.11%	3.624%
2	3.558	93	97	105	rBV	192630	266256	1.79%	0.322%
3	5.381	400	407	419	rBV	4581693	6943288	46.57%	8.390%
4	6.928	660	670	690	rBV	4562384	7525717	50.48%	9.094%
5	7.763	805	812	818	rBV	1146601	1889432	12.67%	2.283%
6	8.904	998	1006	1016	rBV	2976485	4756119	31.90%	5.747%
7	9.463	1092	1101	1109	rBV	129806	203104	1.36%	0.245%
8	10.540	1275	1284	1291	rBV	1676944	2698654	18.10%	3.261%
9	11.275	1401	1409	1418	rBV2	165116	303325	2.03%	0.367%
10	13.004	1695	1703	1710	rBV	7232060	11021176	73.92%	13.317%
11	14.387	1931	1938	1945	rBV	2320336	3476607	23.32%	4.201%
12	15.904	2189	2196	2207	rBV	5105185	7970752	53.46%	9.631%
13	17.198	2409	2416	2420	rBV	2686892	3947461	26.48%	4.770%
14	17.233	2420	2422	2428	rVB	120347	161763	1.09%	0.195%
15	18.151	2572	2578	2587	rBV	885720	1422953	9.54%	1.719%
16	19.327	2773	2778	2782	rBV	330930	508285	3.41%	0.614%
17	19.480	2799	2804	2817	rBV	516493	805390	5.40%	0.973%
18	19.704	2838	2842	2846	rBV	254016	308386	2.07%	0.373%
19	19.933	2874	2881	2891	rVB	10672292	14908664	100.00%	18.015%
20	21.339	3115	3120	3132	rVB	853827	1471826	9.87%	1.778%
21	21.645	3165	3172	3178	rBV2	2239265	4177778	28.02%	5.048%
22	22.604	3330	3335	3345	rVB2	437595	881496	5.91%	1.065%
23	25.010	3736	3744	3752	rVB	1686659	4111111	27.58%	4.968%

Sum of corrected areas: 82758390

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Instrument :
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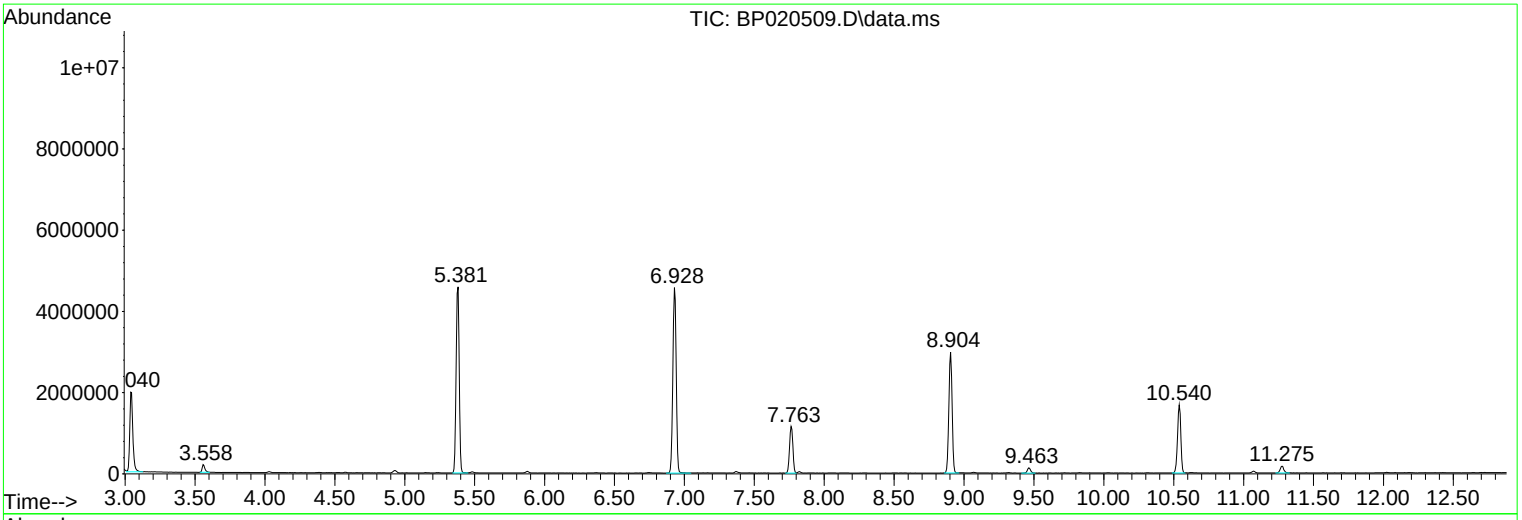
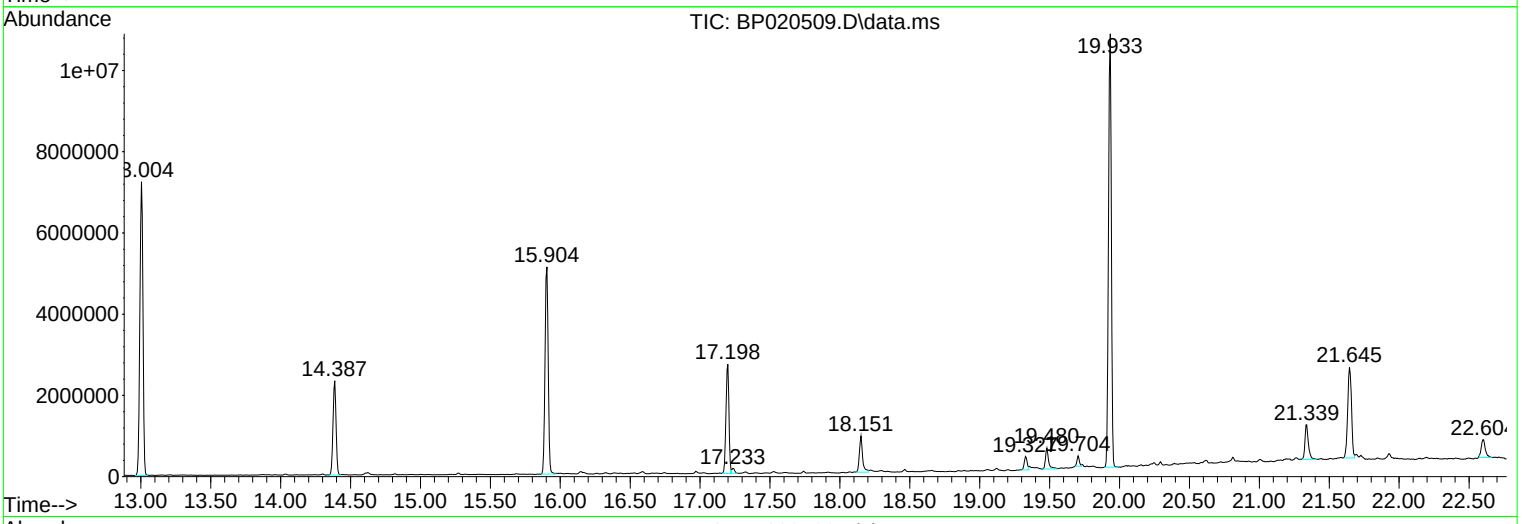
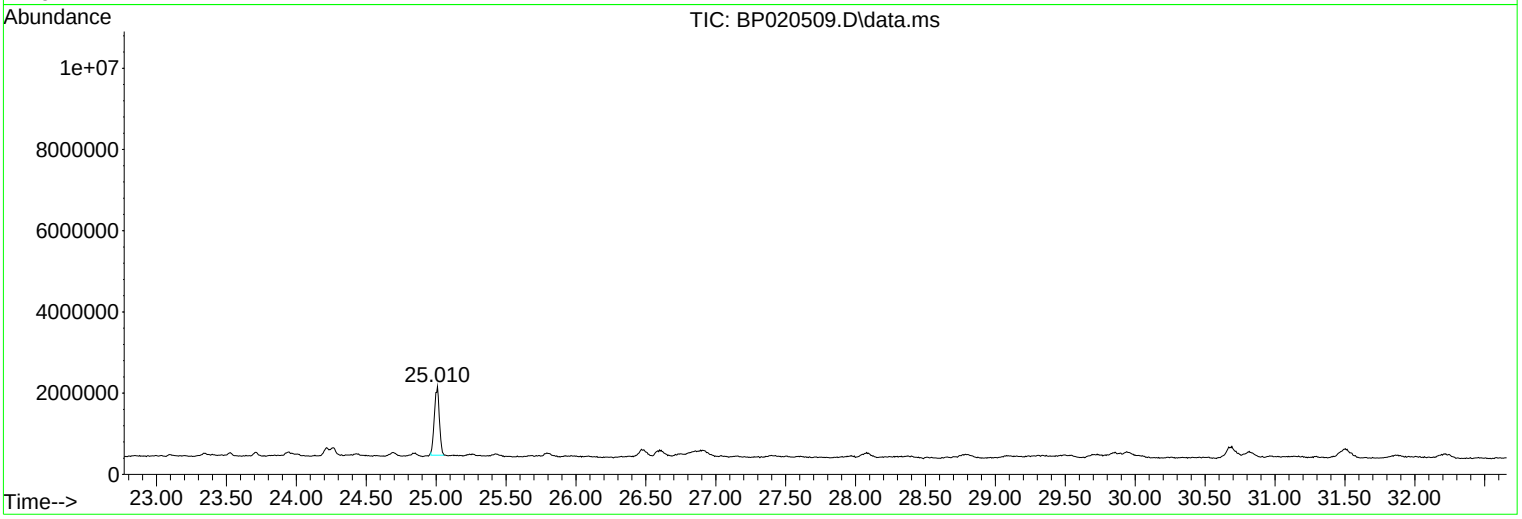
ClientSampleId :
BU-03-05312024

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

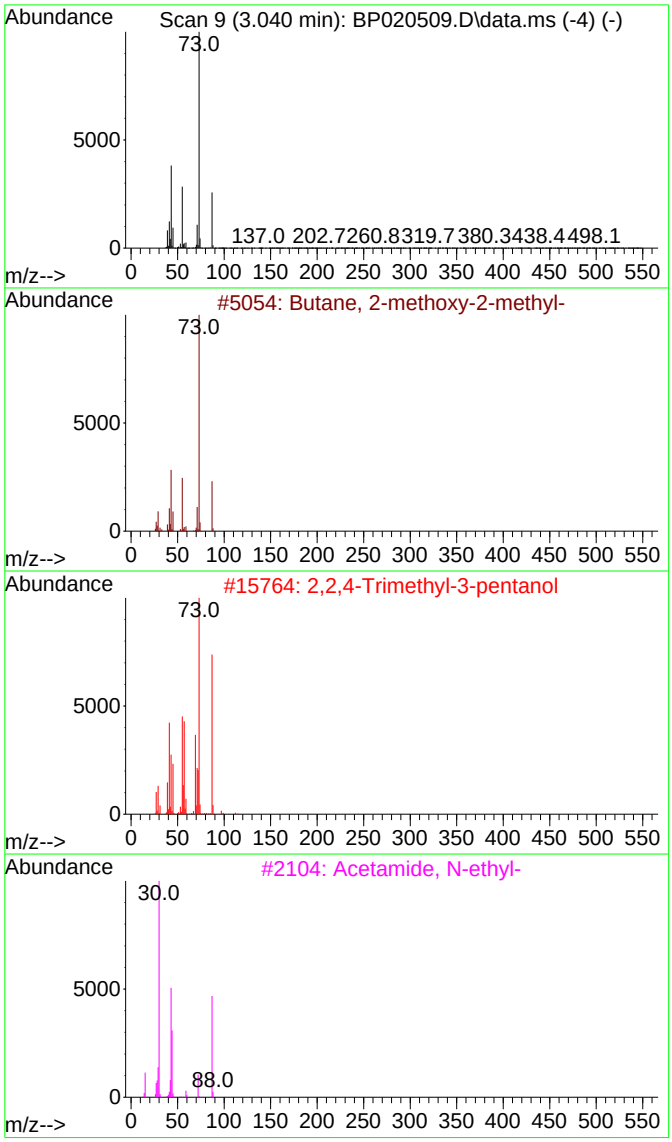
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

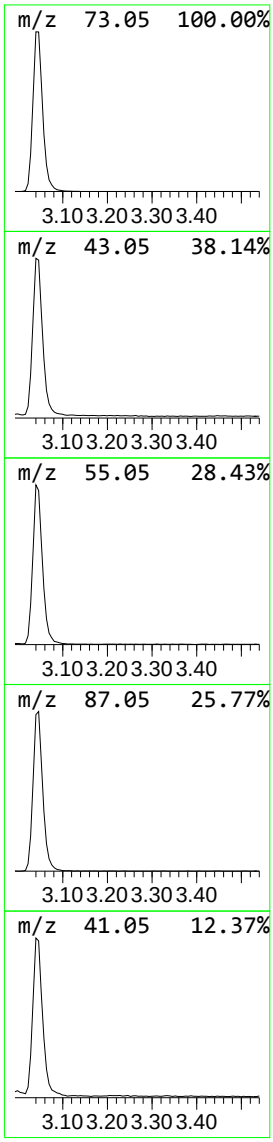
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.040	31.74 ng	2998850	1,4-Dichlorobenzene-d4	7.763

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	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Operator : MA/JU
Sample : P2689-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BU-03-05312024

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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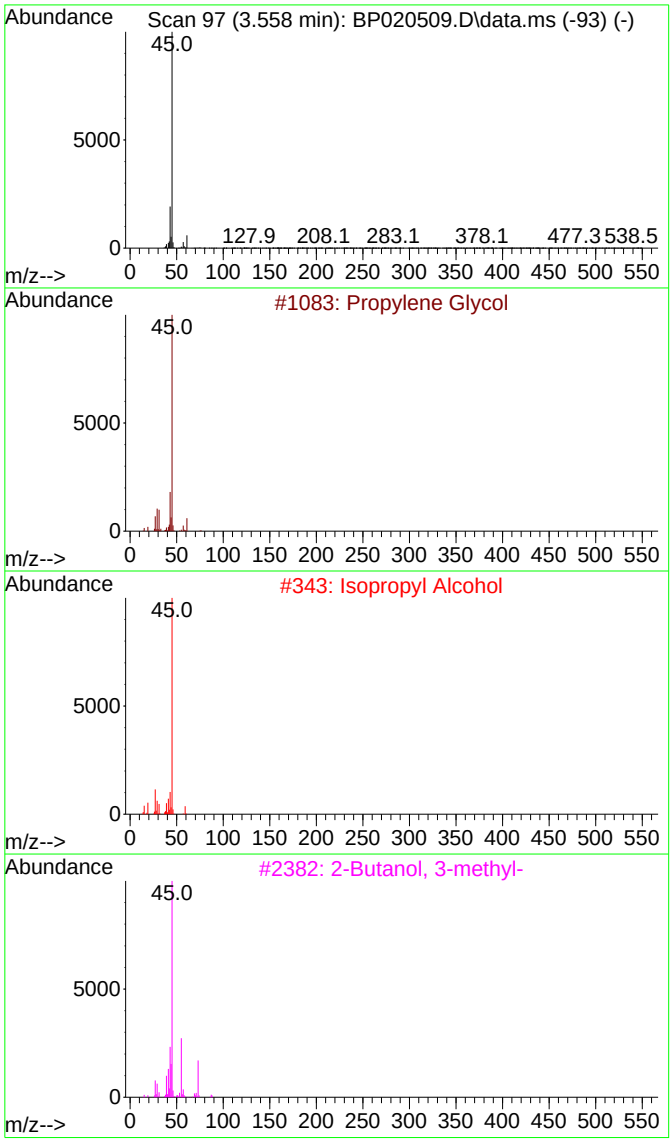
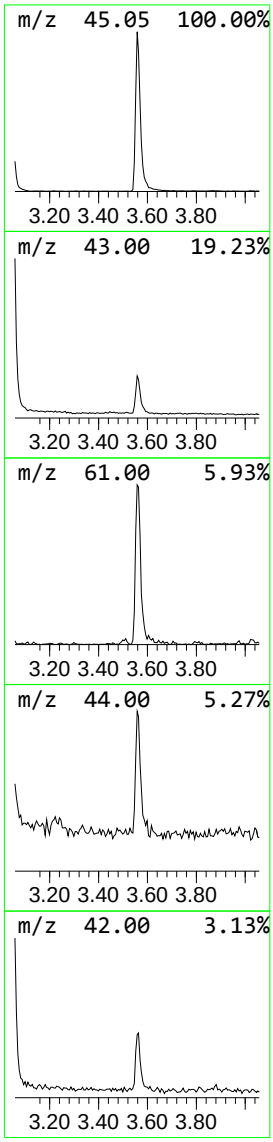
Peak Number 2 unknown3.558 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.558	2.82 ng	266256	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	43
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
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Sample : P2689-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-05312024

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

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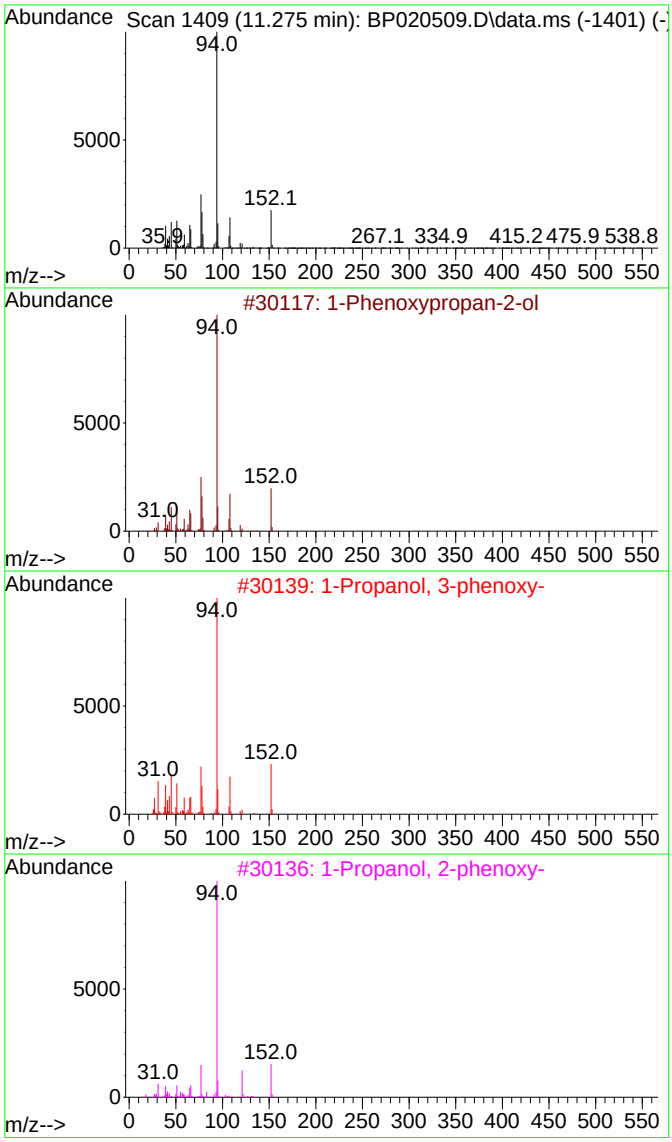
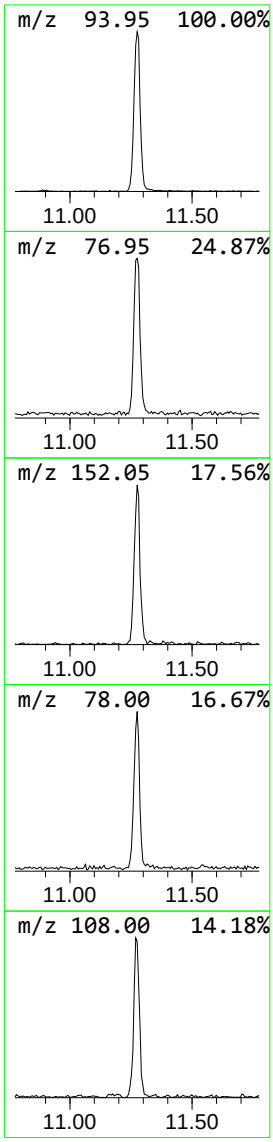
Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.275	2.25 ng	303325	Naphthalene-d8	10.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Carbonic acid, sec-butyl phenyl ...	194	C11H14O3	013183-17-0	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64





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Operator : MA/JU
Sample : P2689-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-05312024

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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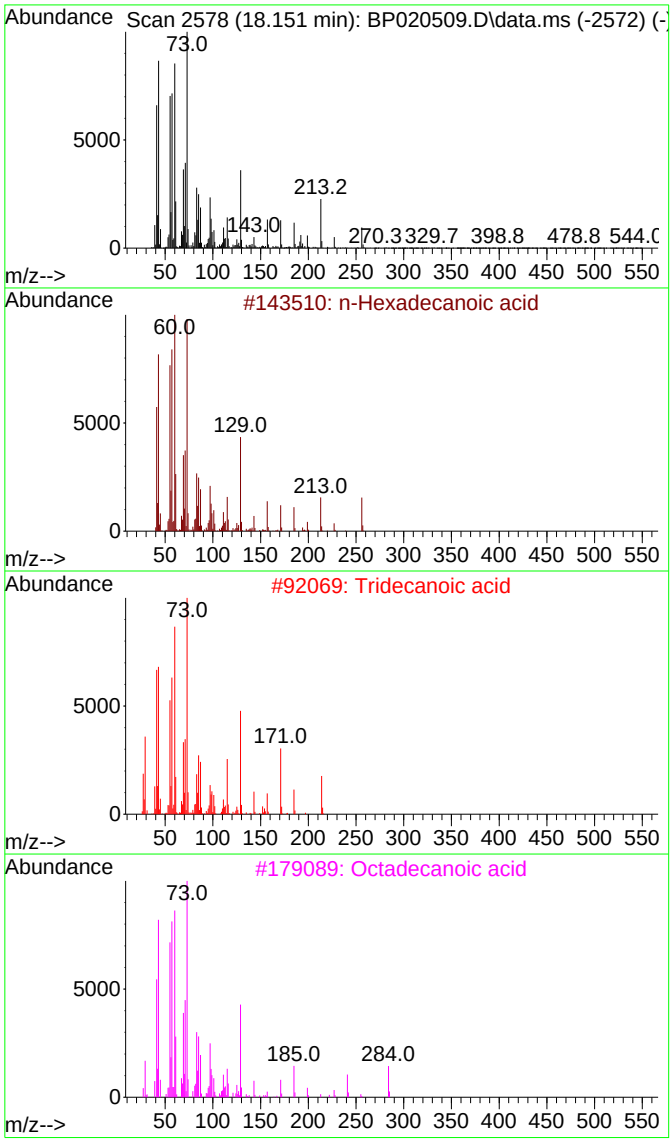
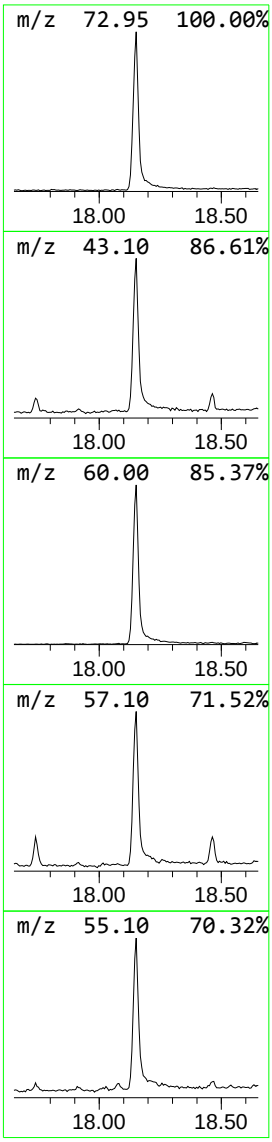
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	7.21 ng	1422950	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	70





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Acq On : 05 Jun 2024 00:06
Operator : MA/JU
Sample : P2689-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
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

TIC Library : C:\Database\NIST20.L
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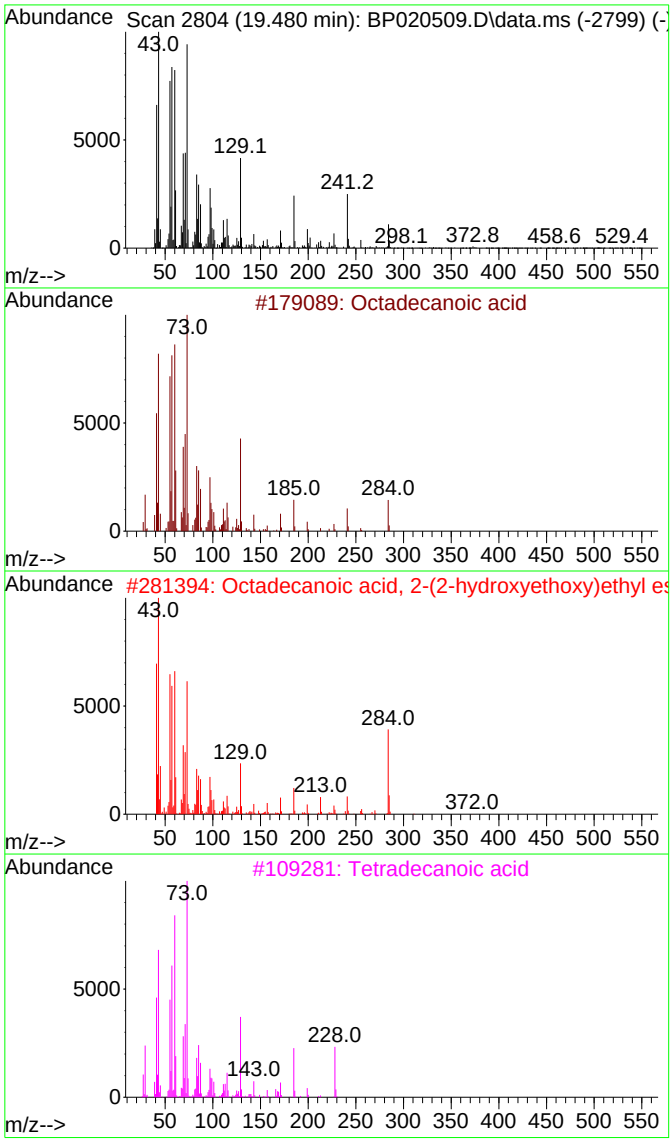
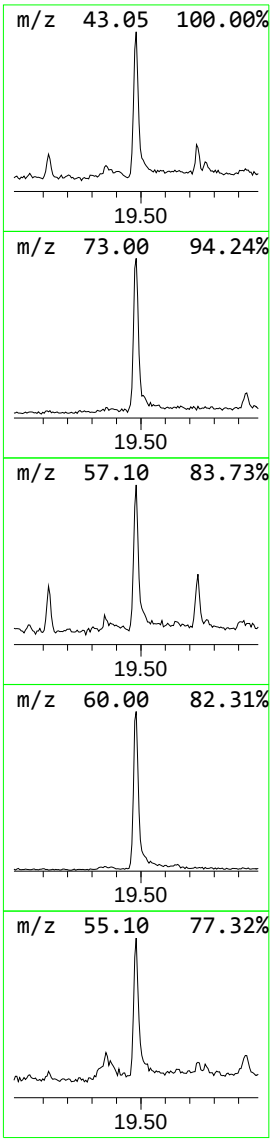
Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.480	3.86 ng	805390	Chrysene-d12	21.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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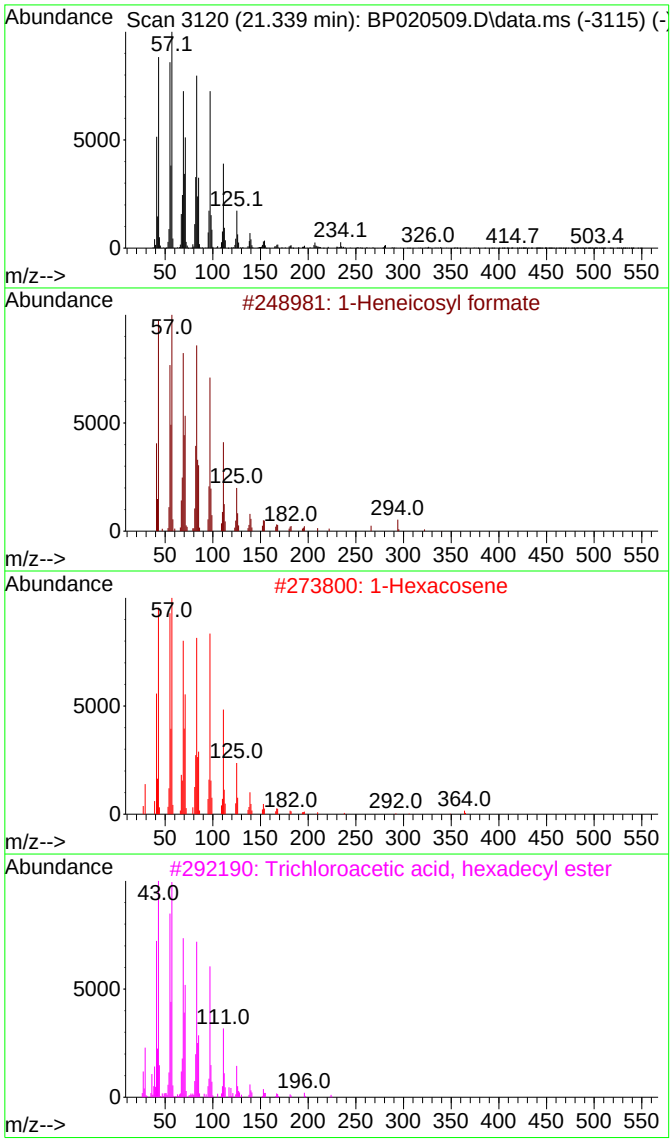
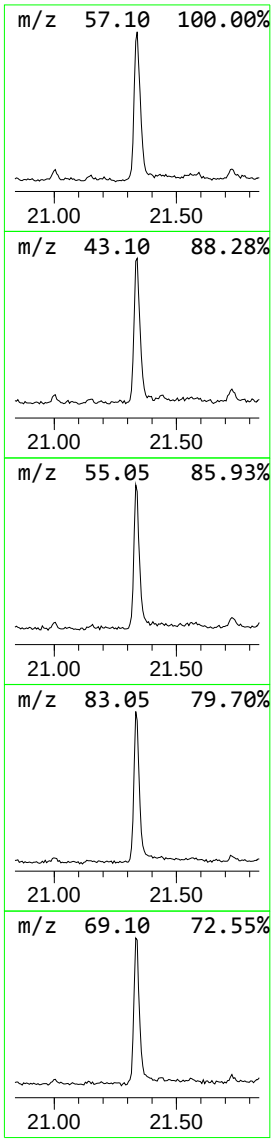
Peak Number 7 1-Heneicosyl formate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.339	7.05 ng	1471830	Chrysene-d12	21.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2	1-Hexacosene	364	C26H52	018835-33-1	95
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	94
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	94





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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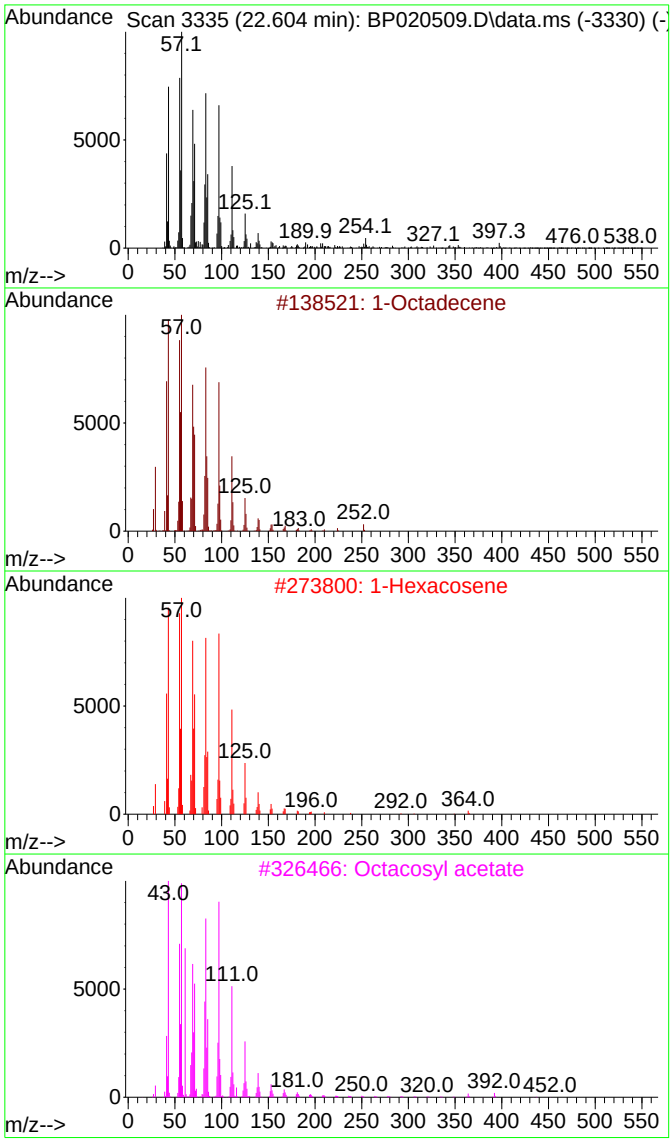
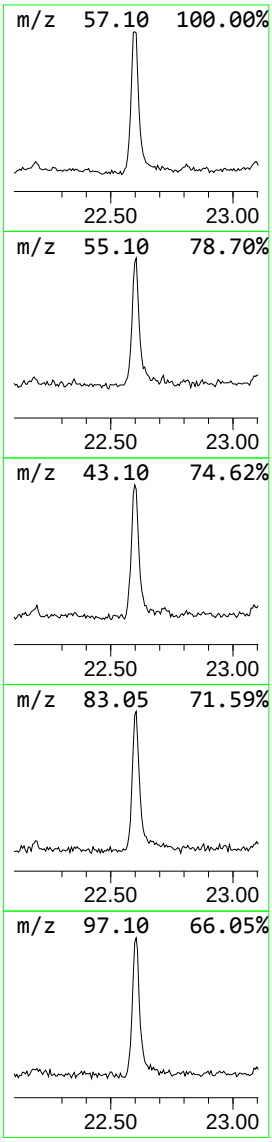
Peak Number 8 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.604	4.22 ng	881496	Chrysene-d12	21.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	94
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	Octacosyl acetate	452	C30H60O2	018206-97-8	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	93





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.040	31.7	ng	2998850	1	7.763	1889430	20.0
unknown3.558	3.558	2.8	ng	266256	1	7.763	1889430	20.0
1-Phenoxypropan...	11.275	2.3	ng	303325	2	10.540	2698650	20.0
n-Hexadecanoic ...	18.151	7.2	ng	1422950	4	17.198	3947460	20.0
Octadecanoic acid	19.480	3.9	ng	805390	5	21.645	4177780	20.0
1-Heneicosyl fo...	21.339	7.0	ng	1471830	5	21.645	4177780	20.0
1-Octadecene	22.604	4.2	ng	881496	5	21.645	4177780	20.0