LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092322\
Data File : BP011783.D
Acq On : 23 Sep 2022 13:30
Operator : CG/JU
Sample : N4609-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DSN003

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-BP092122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011783.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.052	7	11	26	rVB	1061861	1636973	3.76%	2.147%
2	5.475	417	423	437	rVB	658867	1068572	2.45%	1.401%
3	7.075	689	695	711	rVB	465792	838644	1.93%	1.100%
4	9.081	1029	1036	1045	rBV	1083191	1811595	4.16%	2.376%
5	10.504	1272	1278	1298	rBV	581642	1124767	2.58%	1.475%
6	10.728	1309	1316	1327	rVB	440852	783368	1.80%	1.027%
7	13.181	1726	1733	1745	rVB	2901886	4287264	9.84%	5.622%
8	14.557	1958	1967	1980	rBV	774449	1194823	2.74%	1.567%
9	16.045	2214	2220	2230	rBV	2294474	3340432	7.67%	4.380%
10	17.316	2430	2436	2446	rVB	1118409	1584781	3.64%	2.078%
11	17.986	2545	2550	2555	rBV	338953	439911	1.01%	0.577%
12	18.198	2578	2586	2590	rBV	353876	570209	1.31%	0.748%
13	19.110	2738	2741	2754	rVB2	397649	497497	1.14%	0.652%
14	19.869	2865	2870	2881	rBV	6985169	7934834	18.22%	10.405%
15	21.116	3078	3082	3088	rBV2	423877	723469	1.66%	0.949%
16	21.398	3125	3130	3135	rBV	1712461	2198271	5.05%	2.883%
17	21.533	3146	3153	3186	rBV	24117245	43552534	100.00%	57.112%
18	23.845	3540	3546	3558	rVB2	1336747	2670551	6.13%	3.502%

Sum of corrected areas: 76258495

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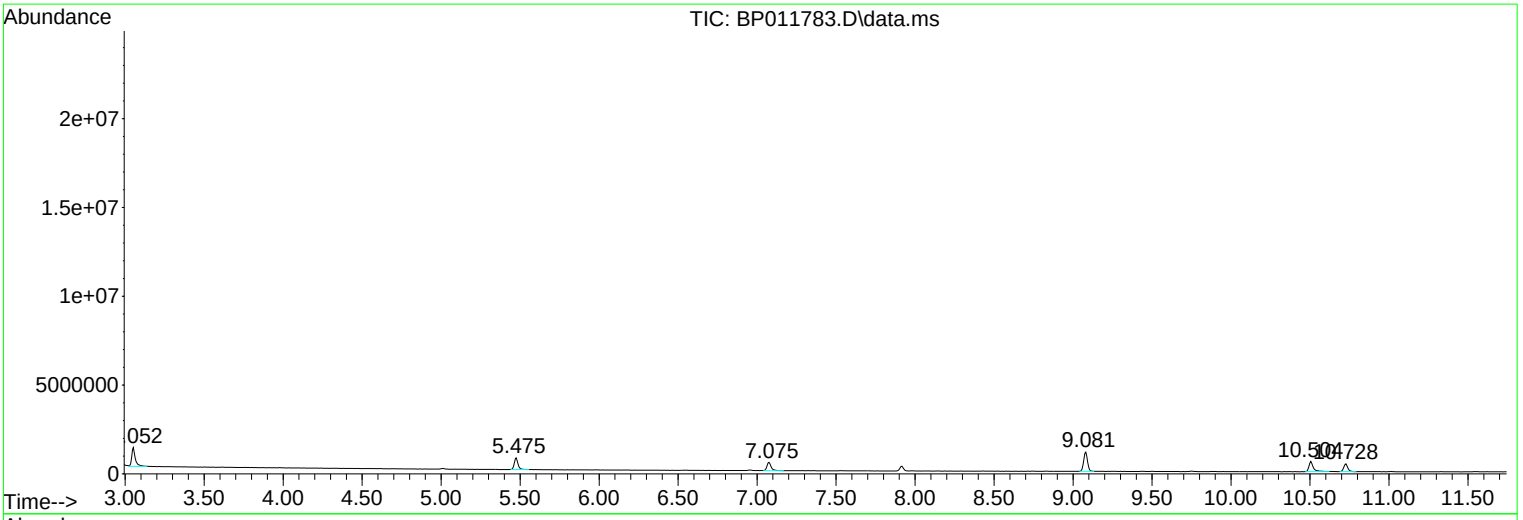
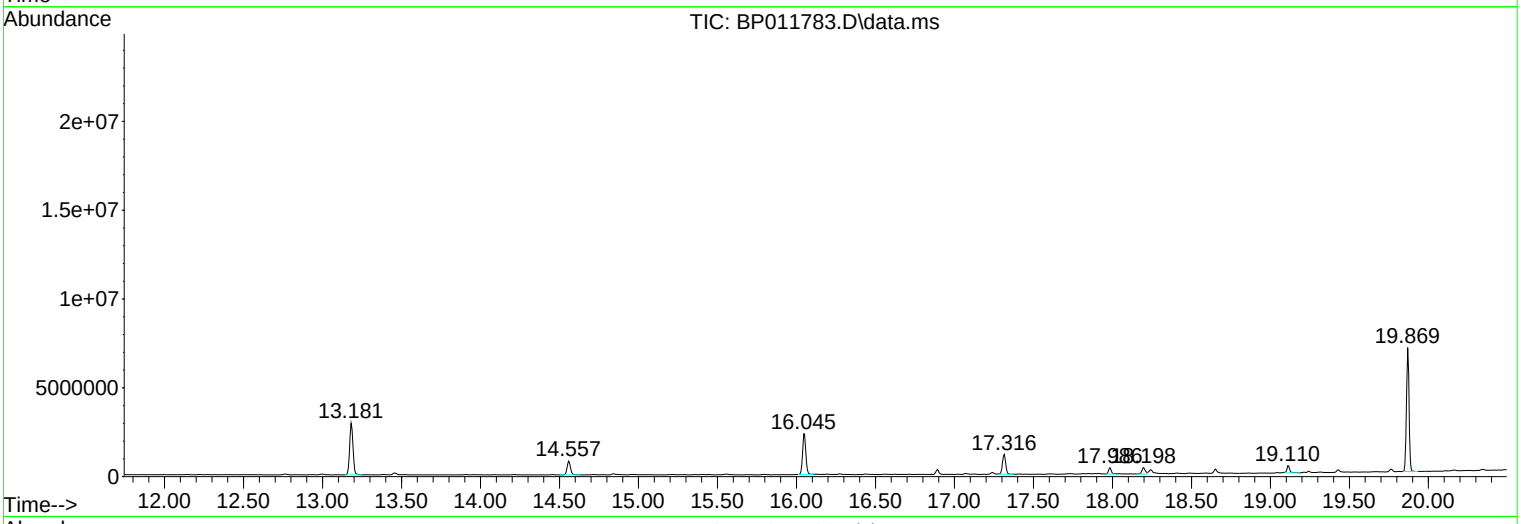
Misc :
ALS Vial : 6 Sample Multiplier: 1

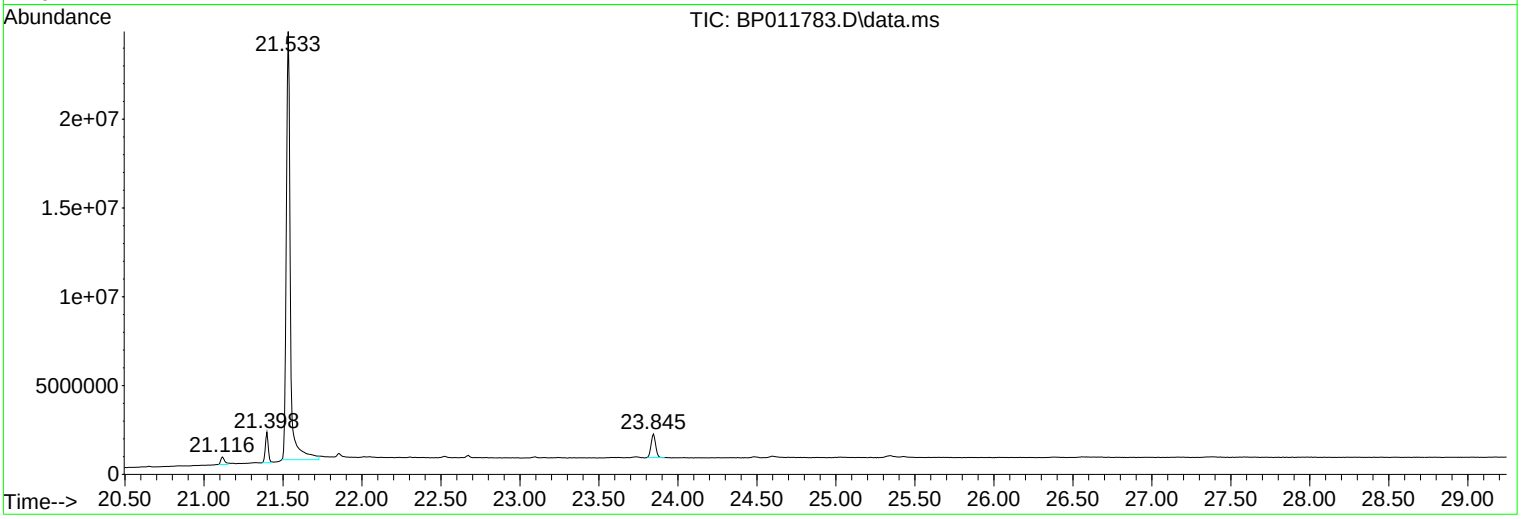
Instrument :
BNA_P
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.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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Data File : BP011783.D
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Operator : CG/JU
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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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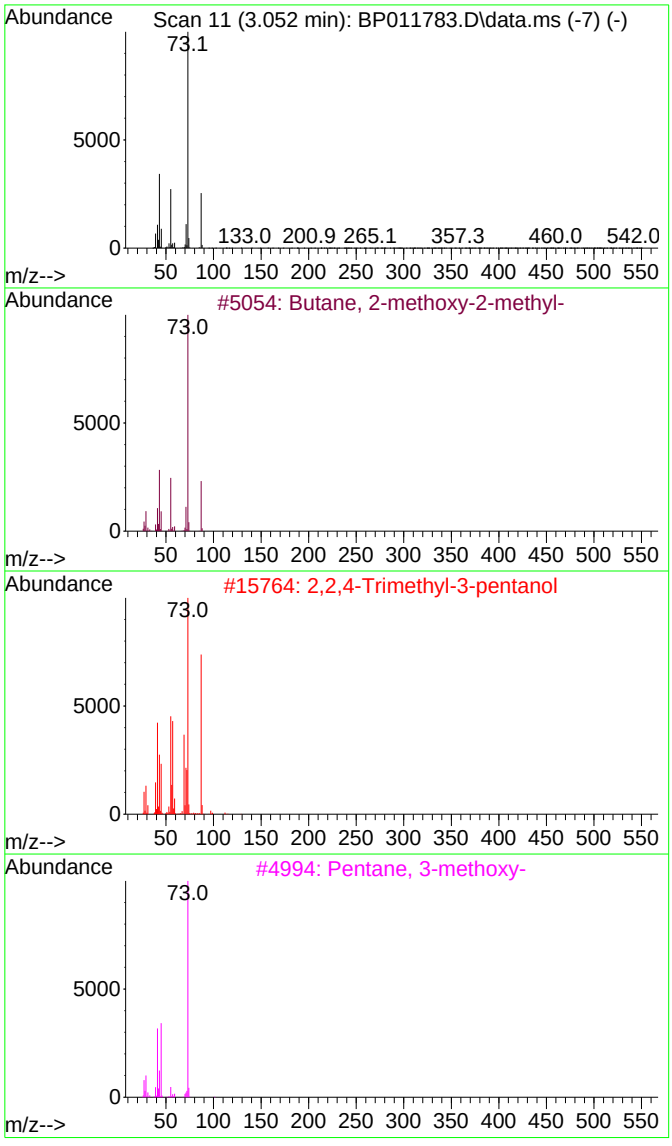
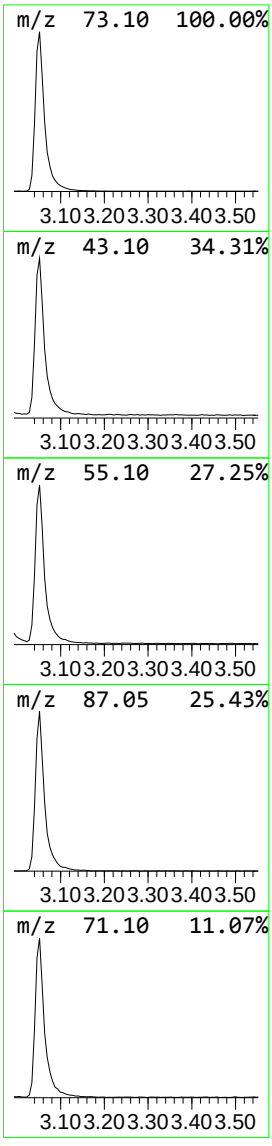
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.052	39.04 ng	1636970	1,4-Dichlorobenzene-d4	7.916

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	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BP011783.D
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Operator : CG/JU
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Instrument :
BNA_P
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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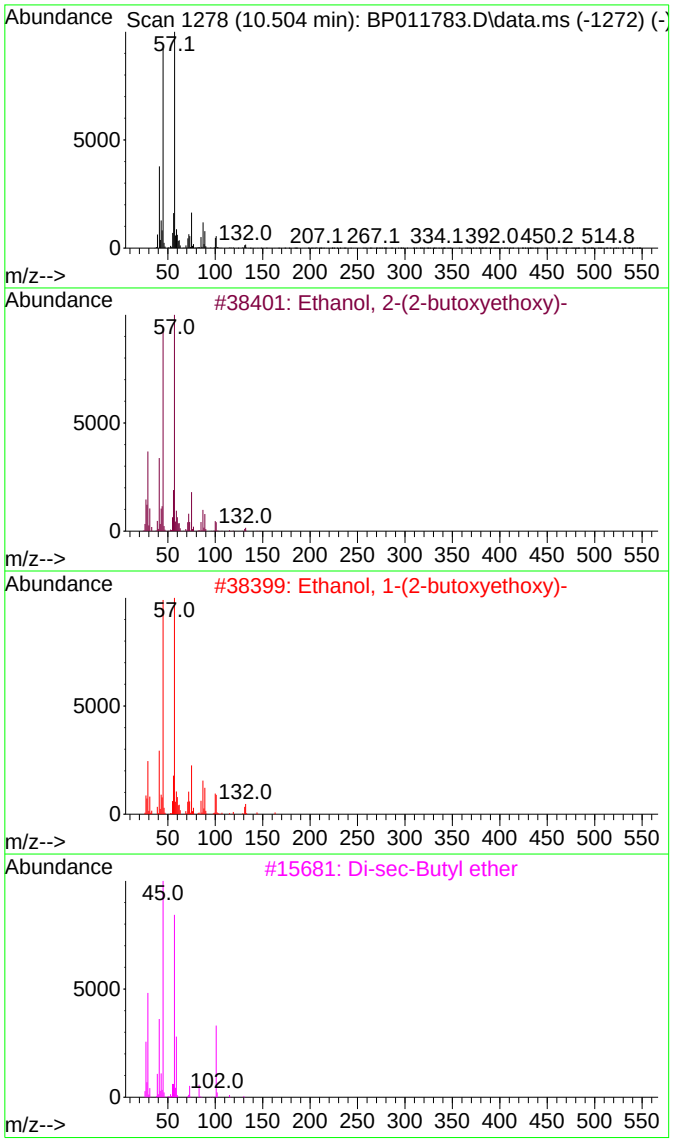
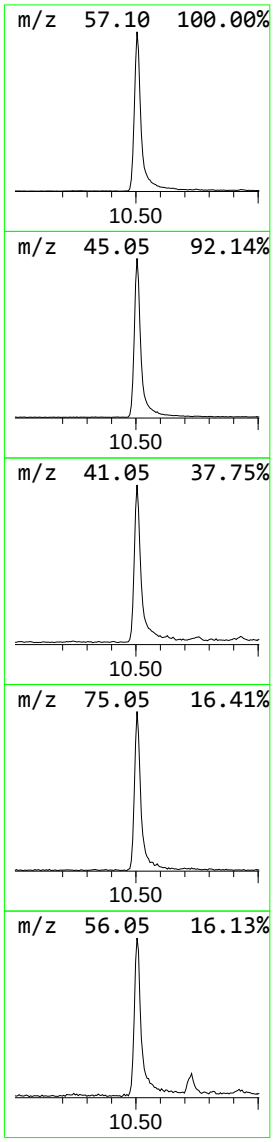
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.504	28.72 ng	1124770	Naphthalene-d8	10.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	53
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50





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Data File : BP011783.D
Acq On : 23 Sep 2022 13:30
Operator : CG/JU
Sample : N4609-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.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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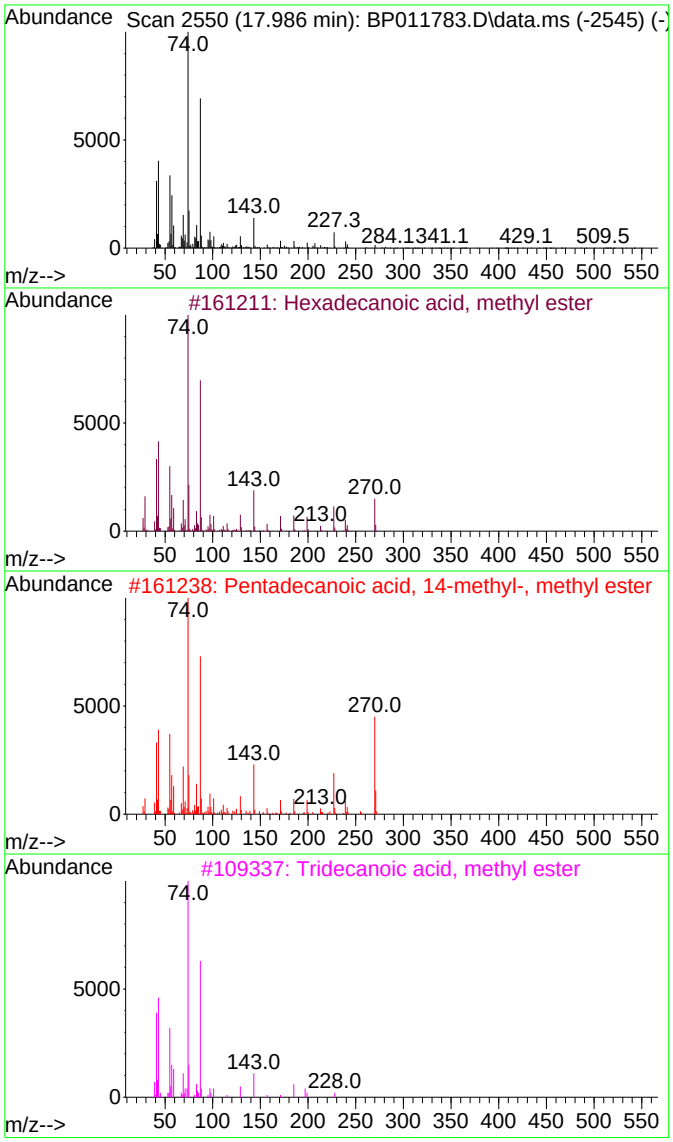
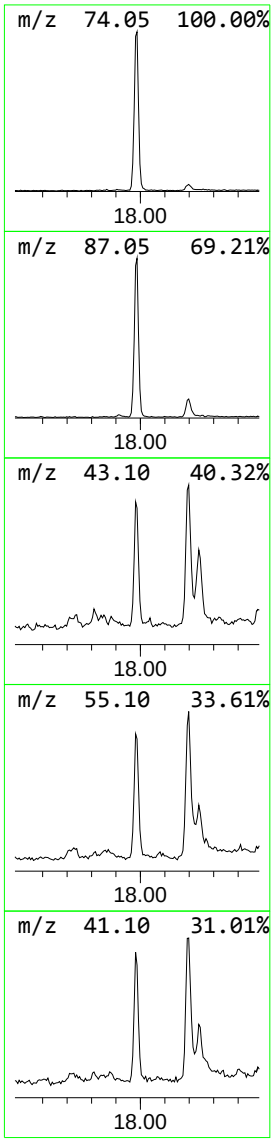
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.986	5.55 ng	439911	Phenanthrene-d10	17.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	92
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	80





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Operator : CG/JU
Sample : N4609-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.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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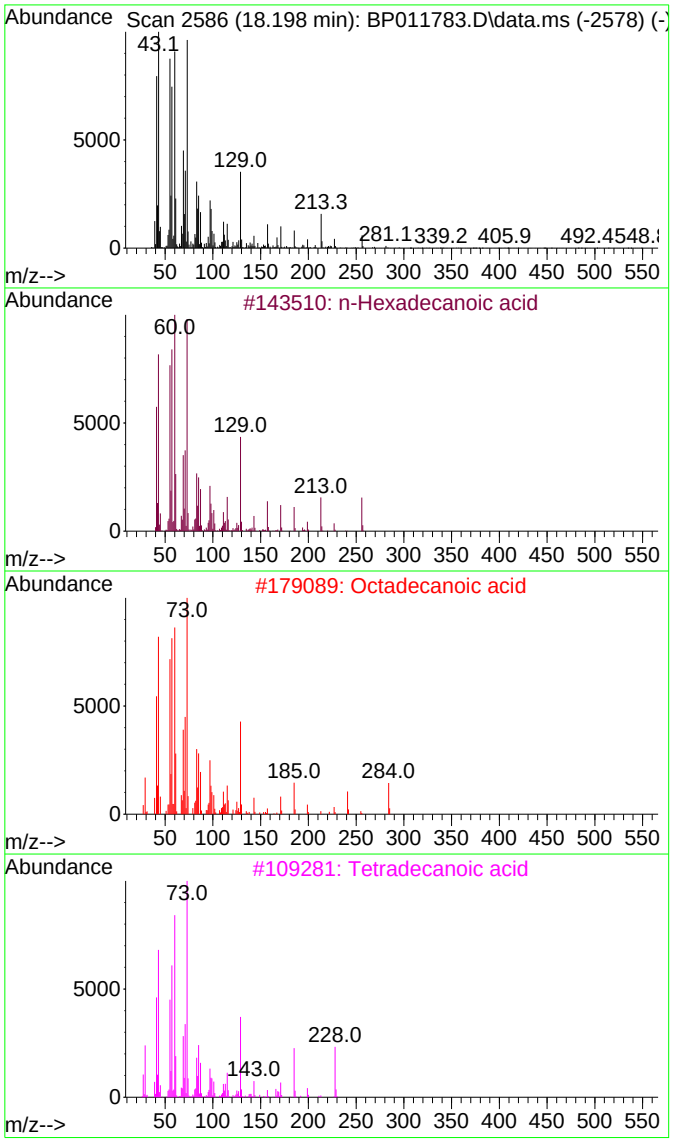
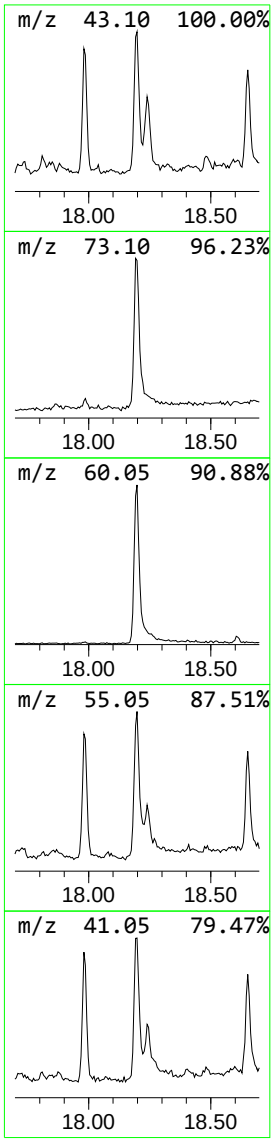
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	7.20 ng	570209	Phenanthrene-d10	17.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Octadecanoic acid	284	C18H36O2	000057-11-4	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





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Data File : BP011783.D
Acq On : 23 Sep 2022 13:30
Operator : CG/JU
Sample : N4609-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

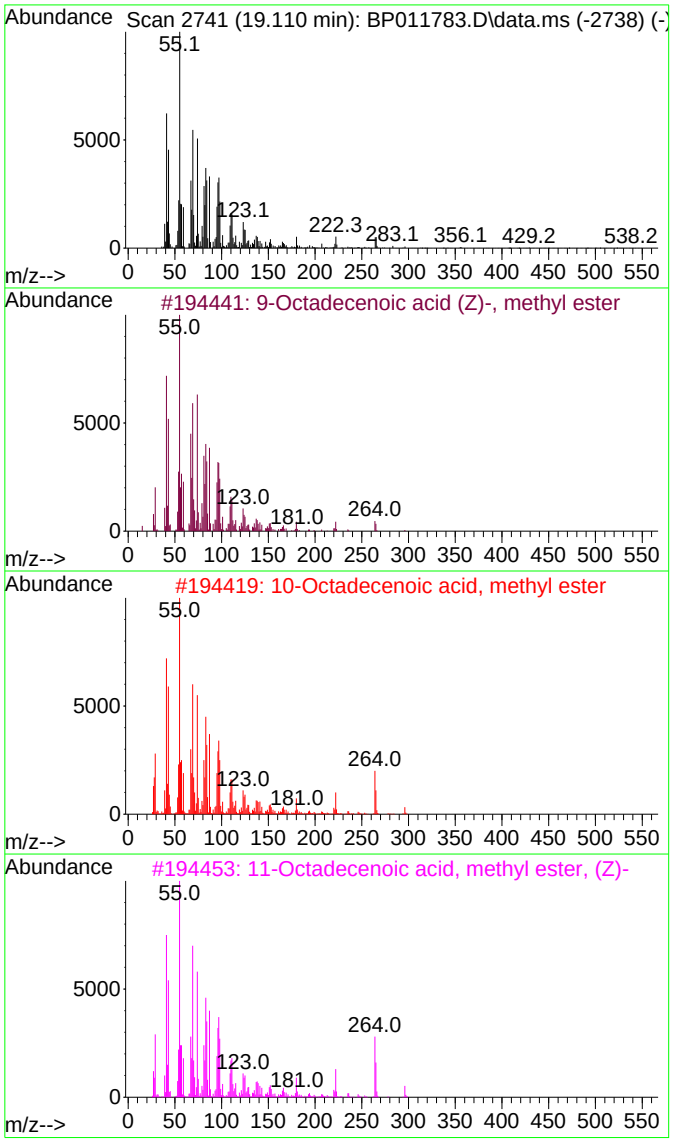
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

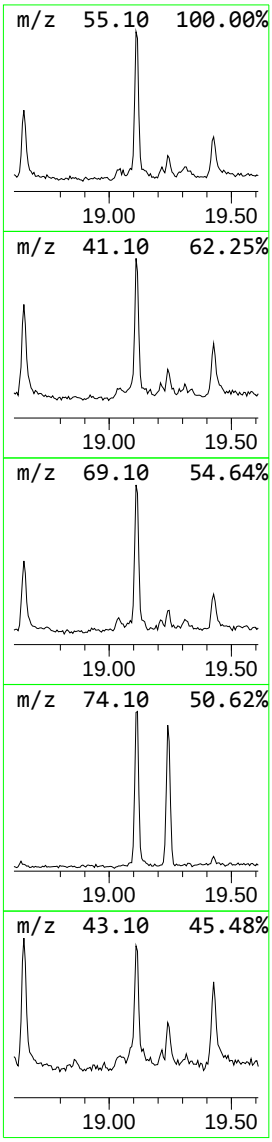
****

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.110	6.28 ng	497497	Phenanthrene-d10	17.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
5	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	99





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Acq On : 23 Sep 2022 13:30
Operator : CG/JU
Sample : N4609-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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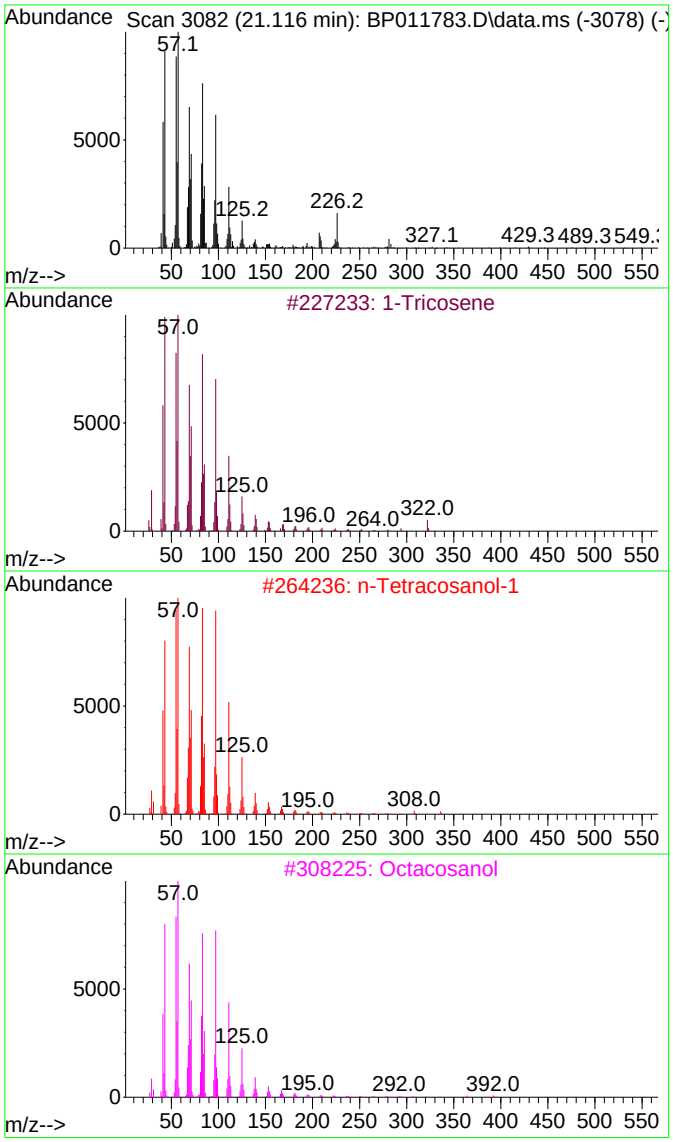
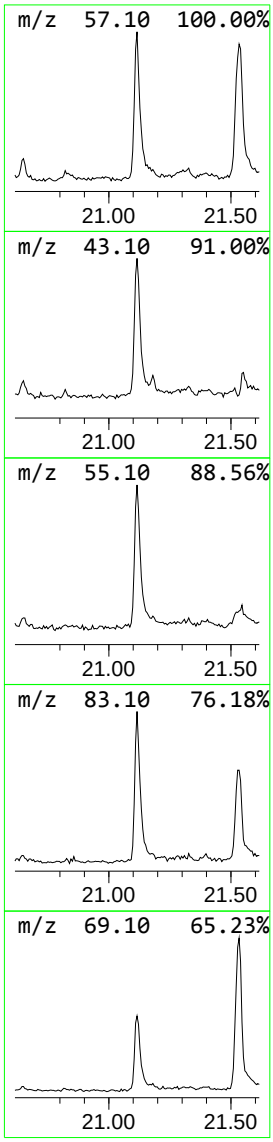
****

Peak Number 6 1-Tricosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.116	6.58 ng	723469	Chrysene-d12	21.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	98
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Octacosanol	410	C28H58O	000557-61-9	94
4	Cyclohexadecane	224	C16H32	000295-65-8	93
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

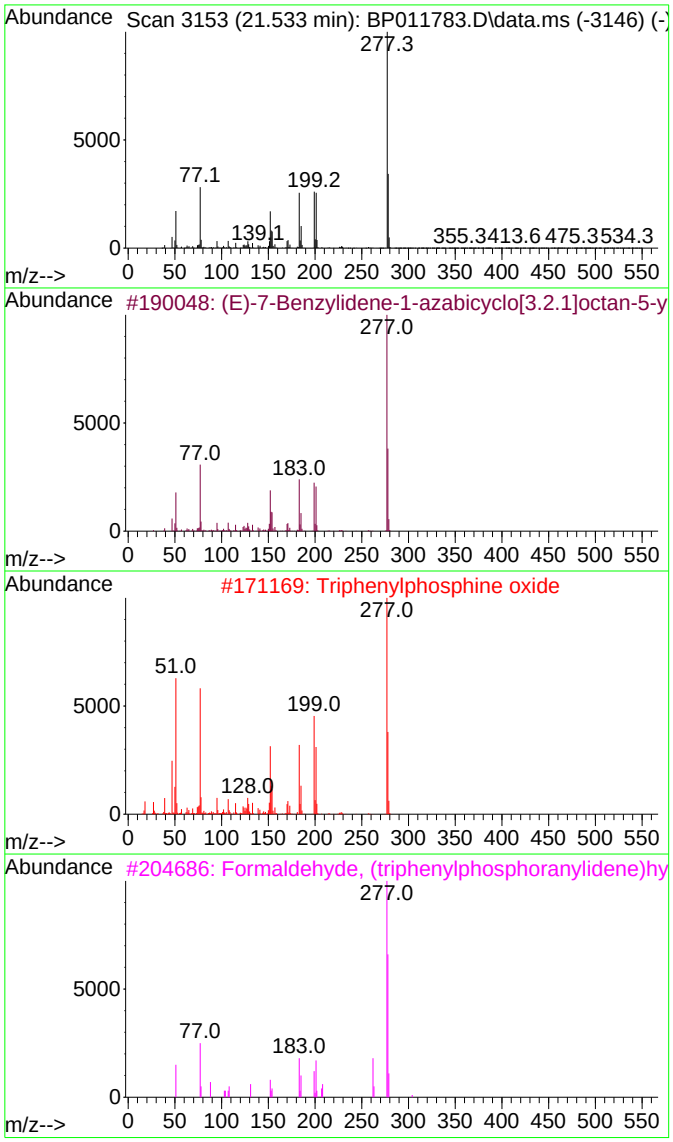
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

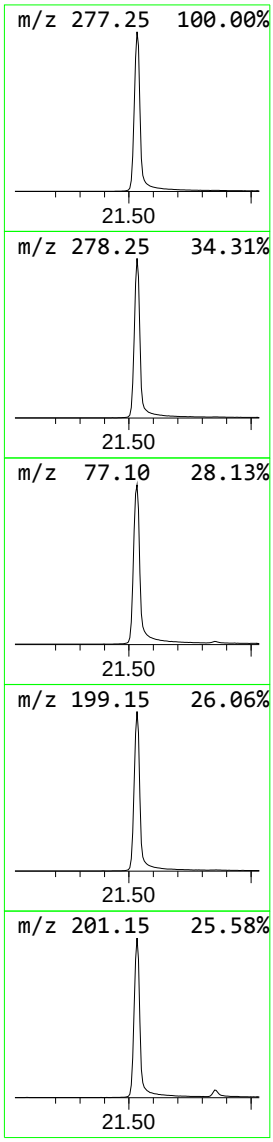
****

Peak Number 7 (E)-7-Benzylidene-1-azabicy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.533	396.24 ng	43552500	Chrysene-d12	21.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	94
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38





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...	3.052	39.0	ng	1636970	1	7.916	838644	20.0
Ethanol, 2-(2-b...	10.504	28.7	ng	1124770	2	10.728	783368	20.0
Hexadecanoic ac...	17.986	5.5	ng	439911	4	17.316	1584780	20.0
n-Hexadecanoic ...	18.198	7.2	ng	570209	4	17.316	1584780	20.0
9-Octadecenoic ...	19.110	6.3	ng	497497	4	17.316	1584780	20.0
1-Tricosene	21.116	6.6	ng	723469	5	21.398	2198270	20.0
(E)-7-Benzylide...	21.533	396.2	ng	43552500	5	21.398	2198270	20.0