LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011222\
Data File : BP008776.D
Acq On : 12 Jan 2022 16:20
Operator : CG/JU
Sample : N1106-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SO-A4-A41-01-6

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-BP010622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008776.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.057	8	12	36	rVB	2571233	3627409	17.36%	3.257%
2	4.981	332	339	346	rBV2	194134	317846	1.52%	0.285%
3	5.446	411	418	433	rBV	5382400	8517065	40.77%	7.646%
4	7.040	681	689	706	rBV	5196554	8943652	42.81%	8.029%
5	7.863	822	829	837	rBV	1560905	2483428	11.89%	2.230%
6	9.022	1018	1026	1046	rBV	3436642	5823150	27.87%	5.228%
7	10.663	1297	1305	1314	rBV	2062501	3509260	16.80%	3.150%
8	13.127	1716	1724	1738	rBV	9880642	14844956	71.06%	13.327%
9	14.504	1951	1958	1971	rBV	3204923	4870287	23.31%	4.372%
10	15.998	2205	2212	2230	rBV	7817980	11528111	55.18%	10.349%
11	17.257	2419	2426	2436	rBV	3857407	5792982	27.73%	5.201%
12	18.151	2573	2578	2592	rBV	416155	692304	3.31%	0.622%
13	19.386	2784	2788	2798	rBV2	177077	341856	1.64%	0.307%
14	19.815	2856	2861	2867	rBV	16728778	20890580	100.00%	18.755%
15	21.056	3068	3072	3079	rBV2	814524	1043403	4.99%	0.937%
16	21.345	3117	3121	3130	rVB	4491027	5575588	26.69%	5.006%
17	21.462	3136	3141	3149	rBV	4658647	7154839	34.25%	6.423%
18	22.609	3333	3336	3342	rVB	533449	797624	3.82%	0.716%
19	23.768	3527	3533	3541	rBV2	2256598	4634148	22.18%	4.160%

Sum of corrected areas: 111388488

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011222\
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Misc :
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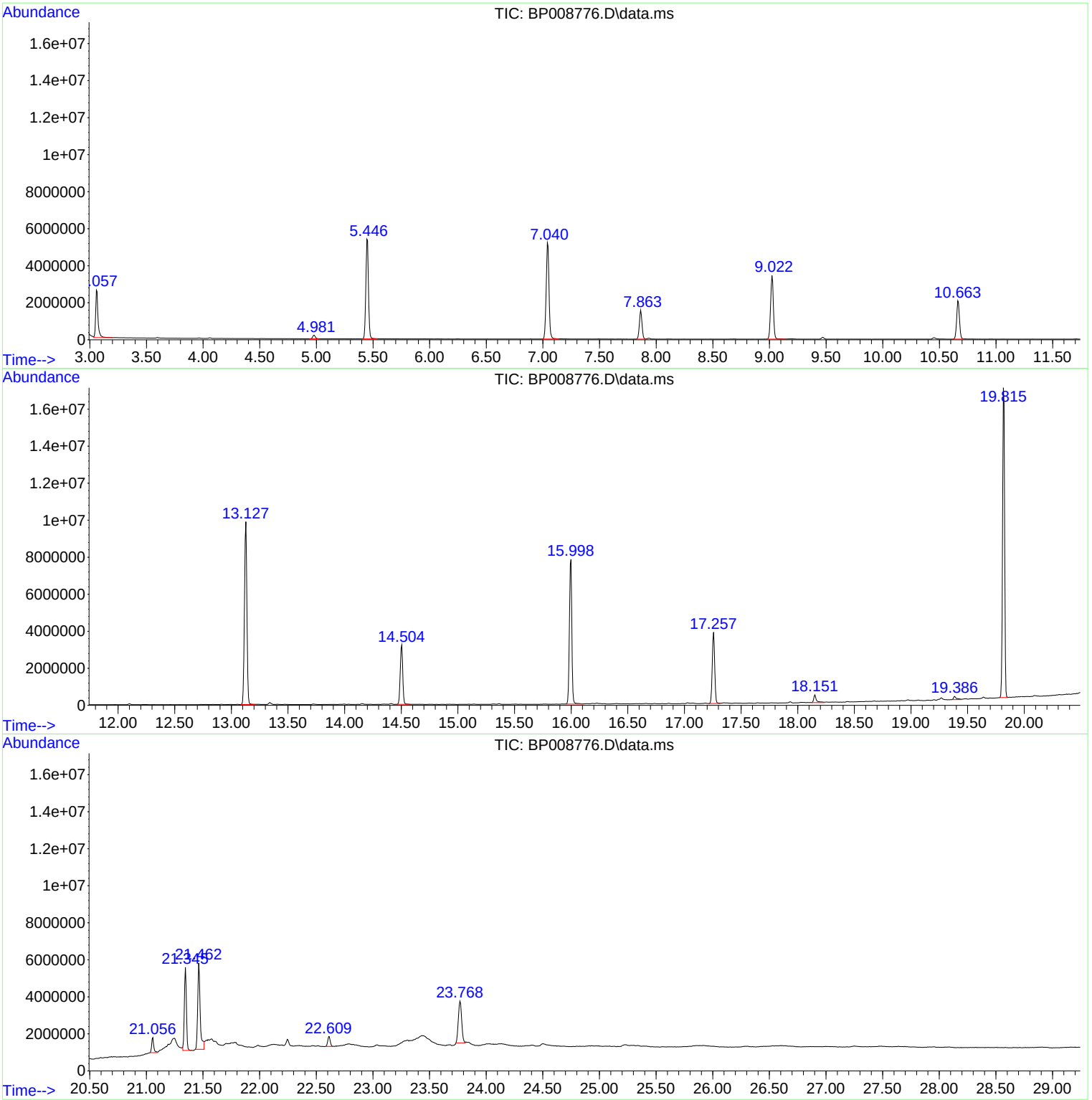
Instrument :
BNA_P
ClientSampleId :
SO-A4-A41-01-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.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\BP011222\
Data File : BP008776.D
Acq On : 12 Jan 2022 16:20
Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

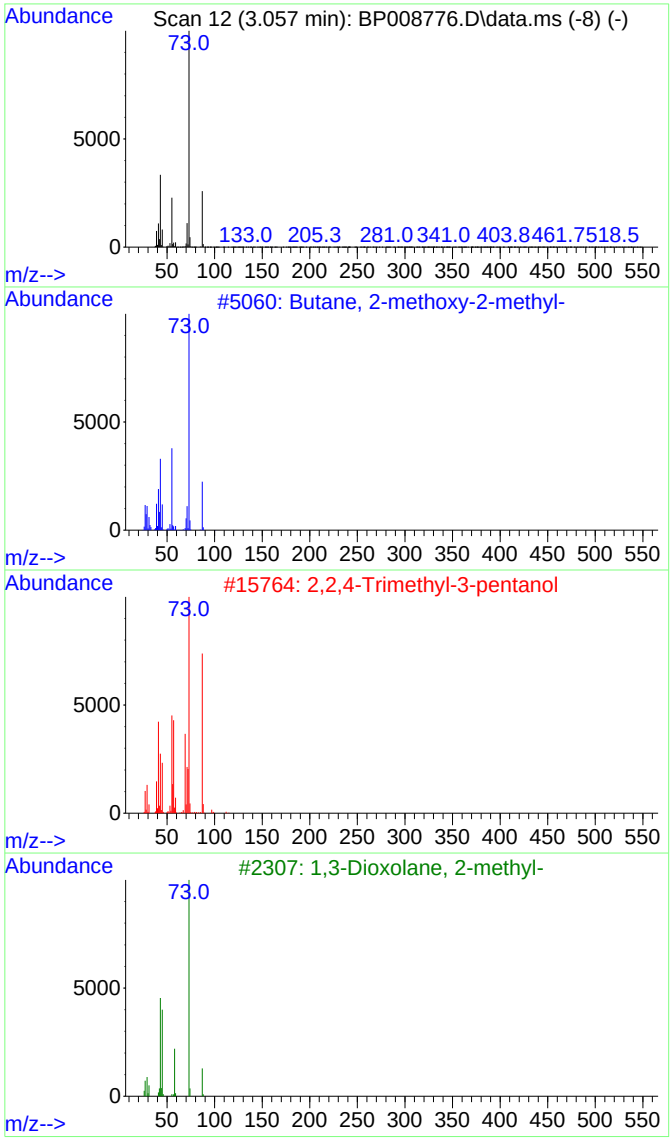
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

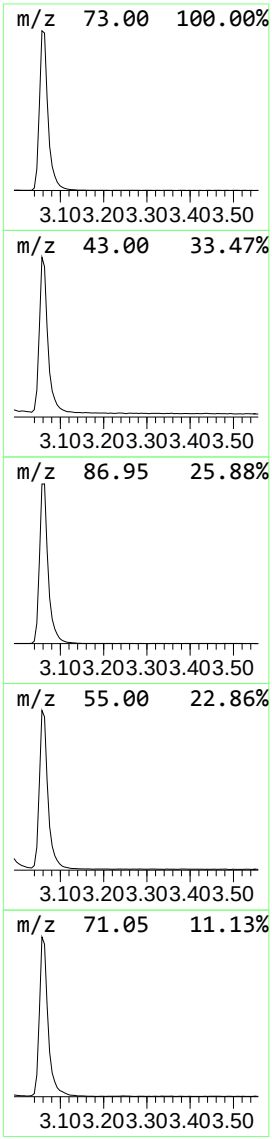
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.057	29.21 ng	3627410	1,4-Dichlorobenzene-d4	7.863

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Data File : BP008776.D
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Operator : CG/JU
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Instrument :
BNA_P
ClientSampleId :
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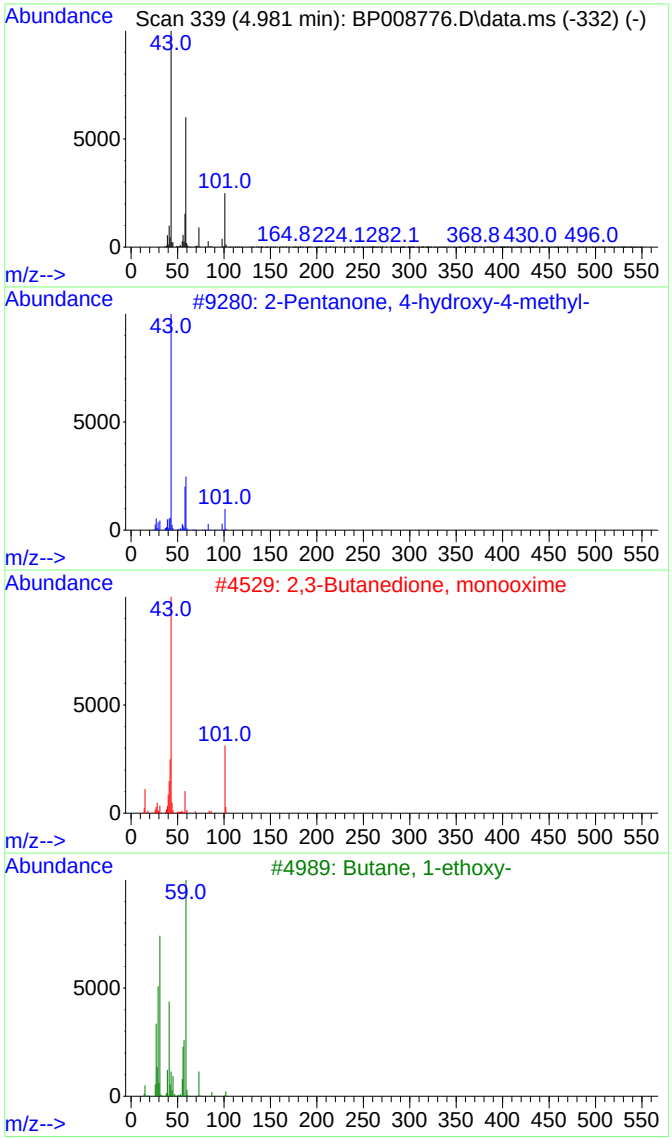
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

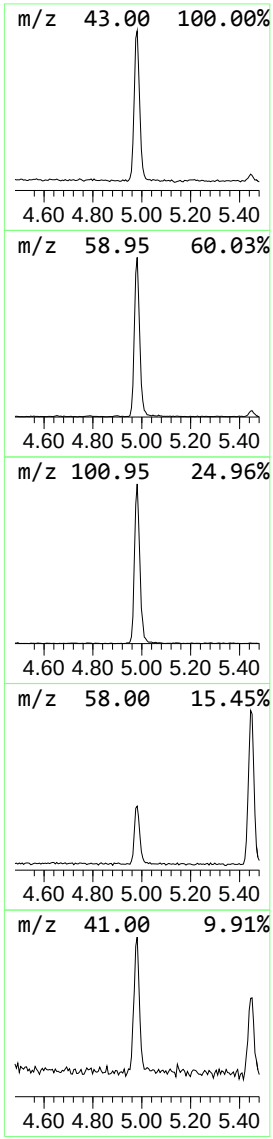
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	2.56 ng	317846	1,4-Dichlorobenzene-d4	7.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	25
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	17





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Data File : BP008776.D
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Operator : CG/JU
Sample : N1106-12
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SO-A4-A41-01-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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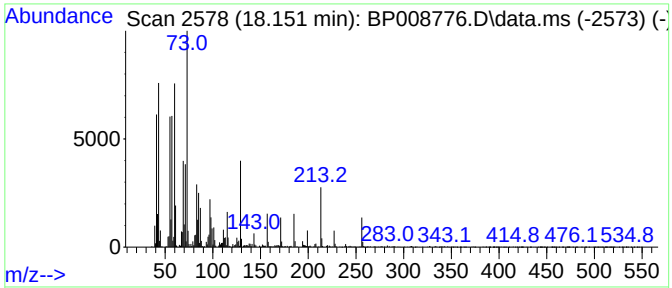
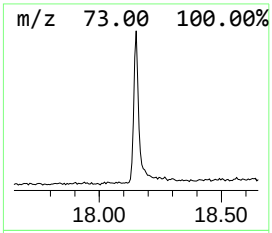
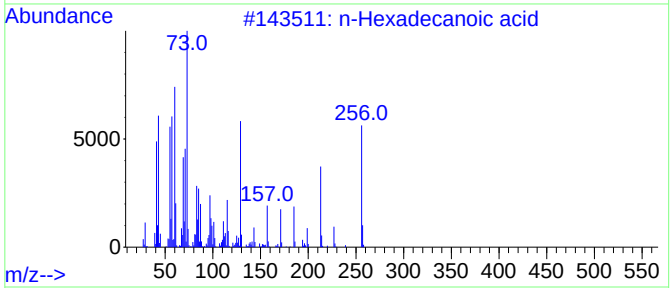
Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

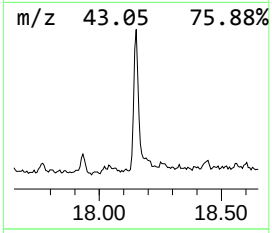
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	2.39 ng	692304	Phenanthrene-d10	17.257

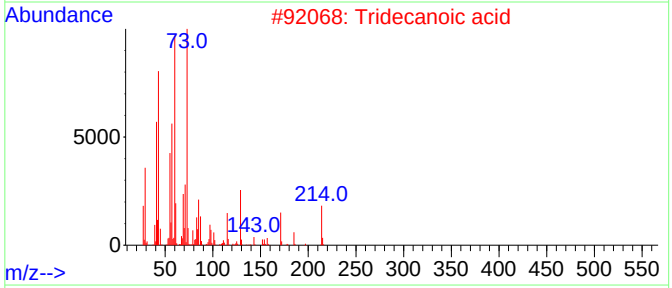
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	83

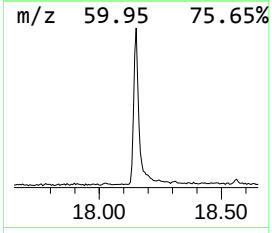


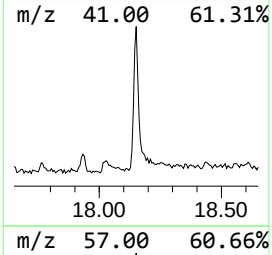


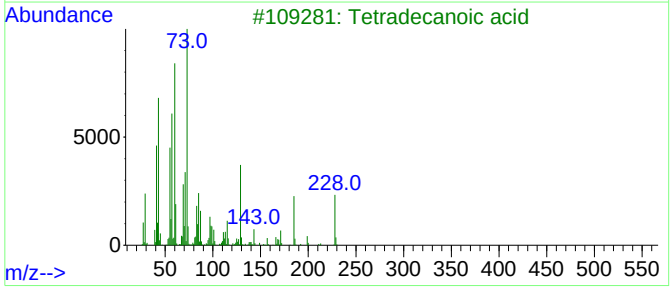


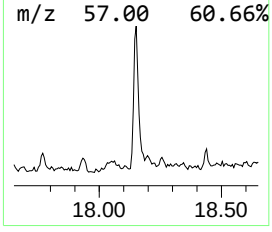












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011222\
Data File : BP008776.D
Acq On : 12 Jan 2022 16:20
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Sample : N1106-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
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SO-A4-A41-01-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

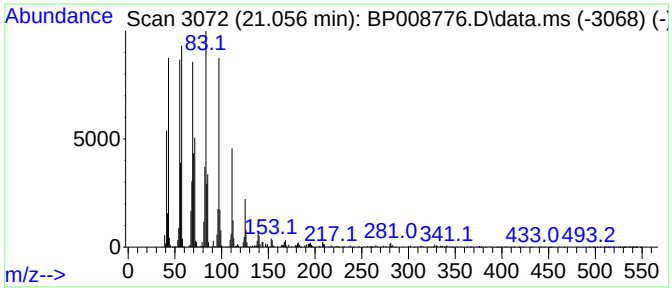
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

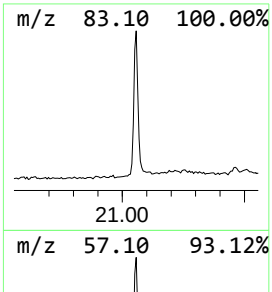
****

Peak Number 4 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.057	3.74 ng	1043400	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Nonacos-1-ene	406	C29H58	018835-35-3	94
4	1-Tetracosene	336	C24H48	010192-32-2	94
5	1-Hexacosene	364	C26H52	018835-33-1	94





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SO-A4-A41-01-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

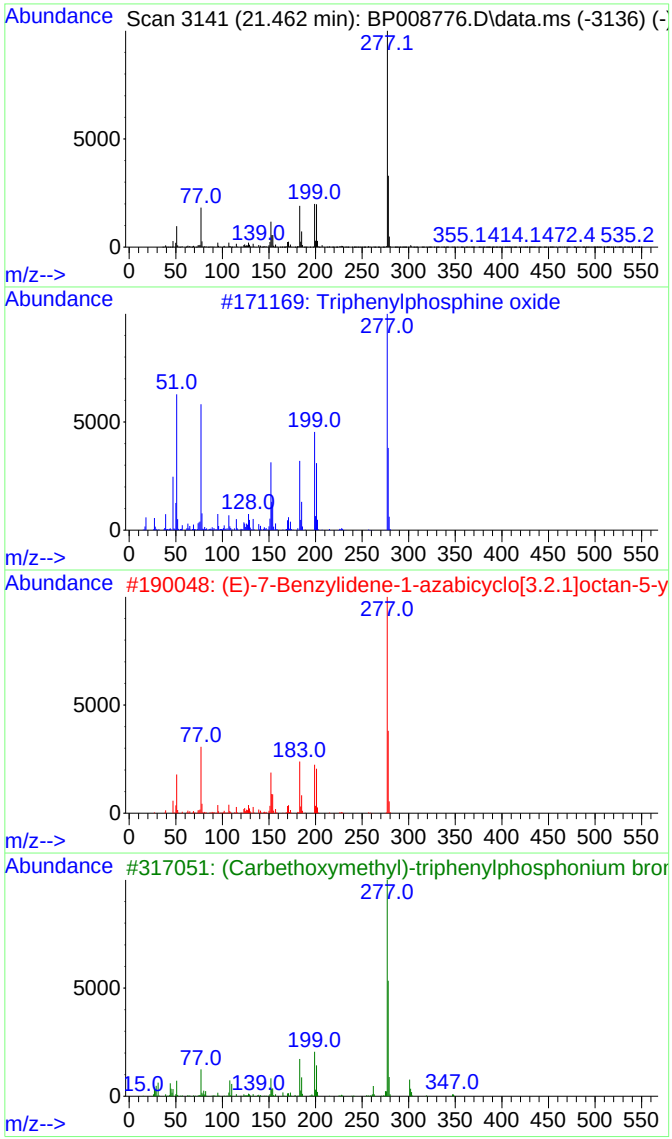
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

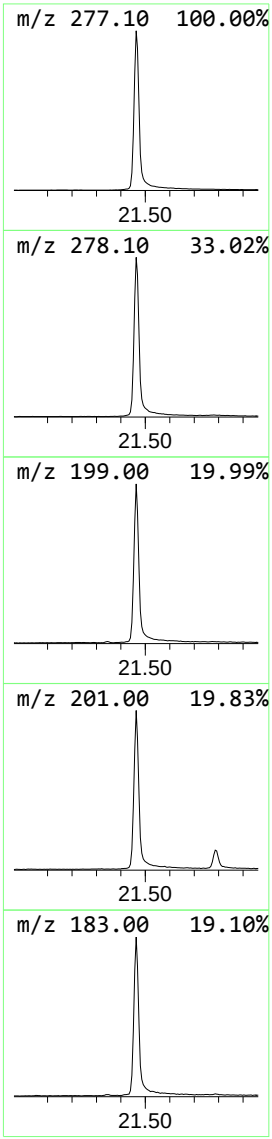
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.462	25.66 ng	7154840	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	92
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	40
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	28





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

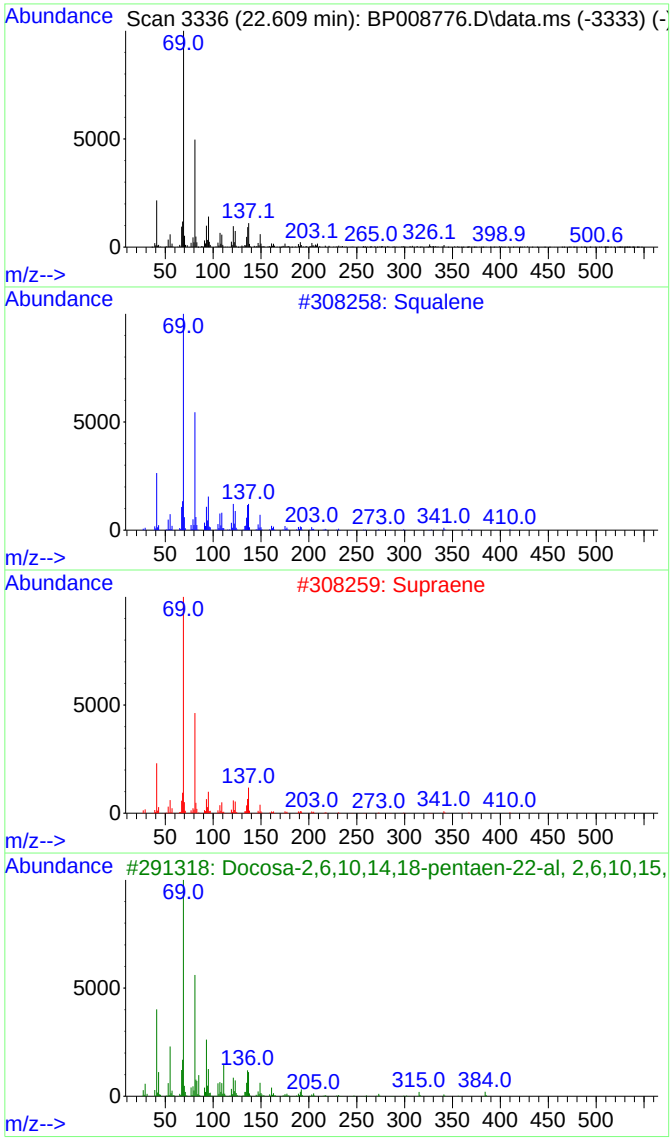
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

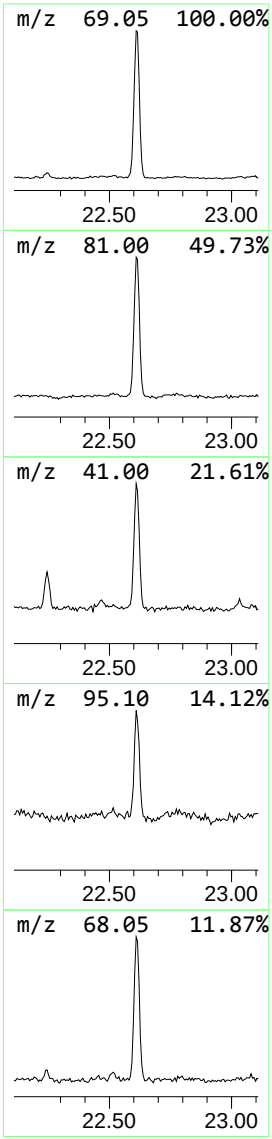
****

Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.609	3.44 ng	797624	Perylene-d12	23.768

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	76
5	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	64





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...	3.057	29.2	ng	3627410	1	7.863	2483430	20.0
2-Pentanone, 4-...	4.981	2.6	ng	317846	1	7.863	2483430	20.0
n-Hexadecanoic ...	18.151	2.4	ng	692304	4	17.257	5792980	20.0
Behenic alcohol	21.057	3.7	ng	1043400	5	21.345	5575590	20.0
Triphenylphosph...	21.462	25.7	ng	7154840	5	21.345	5575590	20.0
Squalene	22.609	3.4	ng	797624	6	23.768	4634150	20.0