LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111222\
Data File : BP012638.D
Acq On : 13 Nov 2022 01:57
Operator : CG/JU
Sample : N5530-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-11

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-BP111222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP012638.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.228	206	211	222	rVB	152582	219798	1.19%	0.243%
2	4.834	308	314	326	rBV	1391205	2016957	10.89%	2.229%
3	5.293	386	392	414	rBV	5071531	7768063	41.94%	8.584%
4	6.899	658	665	686	rBV	5098254	8365055	45.16%	9.244%
5	7.710	794	803	813	rBV	982550	1619972	8.75%	1.790%
6	8.881	994	1002	1021	rBV	3200893	5285664	28.53%	5.841%
7	10.304	1238	1244	1259	rBV	110360	305107	1.65%	0.337%
8	10.504	1271	1278	1294	rBV	1396104	2387278	12.89%	2.638%
9	12.987	1692	1700	1723	rBV	8161313	12813058	69.17%	14.159%
10	14.369	1928	1935	1947	rBV	2282449	3436584	18.55%	3.798%
11	15.869	2180	2190	2208	rBV	7908036	11535606	62.28%	12.748%
12	17.128	2398	2404	2418	rBV	2910019	4248611	22.94%	4.695%
13	18.028	2552	2557	2566	rBV	418106	673948	3.64%	0.745%
14	19.263	2763	2767	2778	rBV	334000	506333	2.73%	0.560%
15	19.704	2836	2842	2855	rBV	14003856	18523626	100.00%	20.470%
16	20.945	3049	3053	3064	rBV4	242908	768283	4.15%	0.849%
17	21.233	3097	3102	3108	rBV	3837184	4779291	25.80%	5.281%
18	22.345	3288	3291	3302	rVB	311554	600768	3.24%	0.664%
19	23.574	3494	3500	3512	rVB2	2361518	4637356	25.03%	5.125%

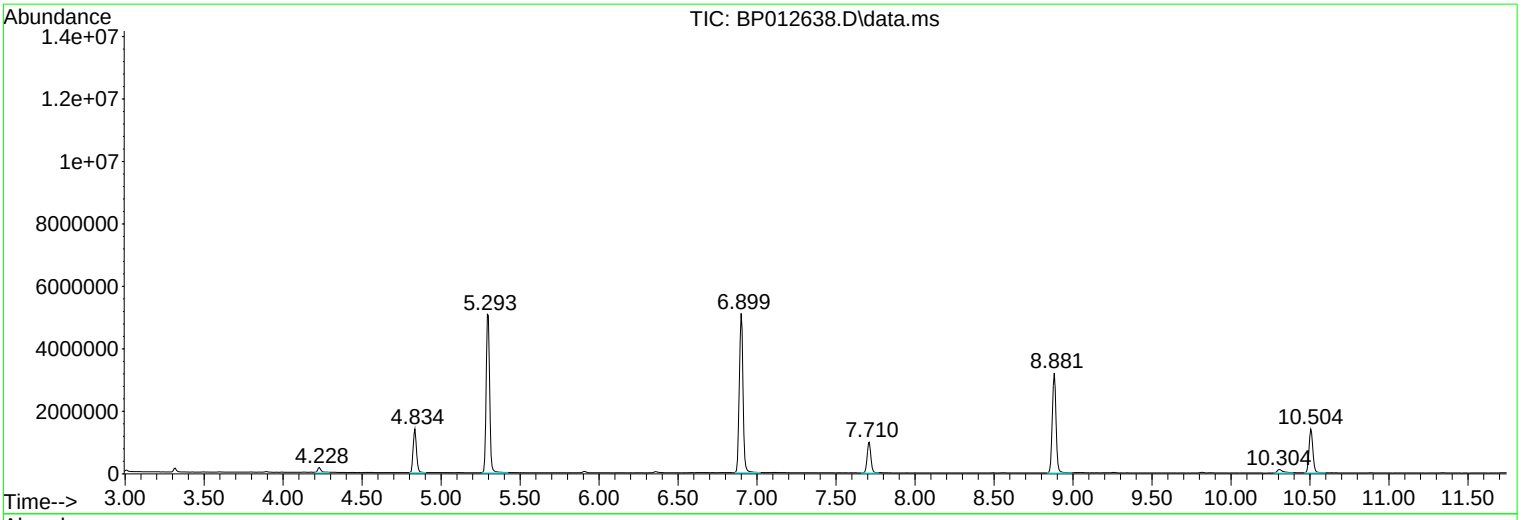
Sum of corrected areas: 90491358

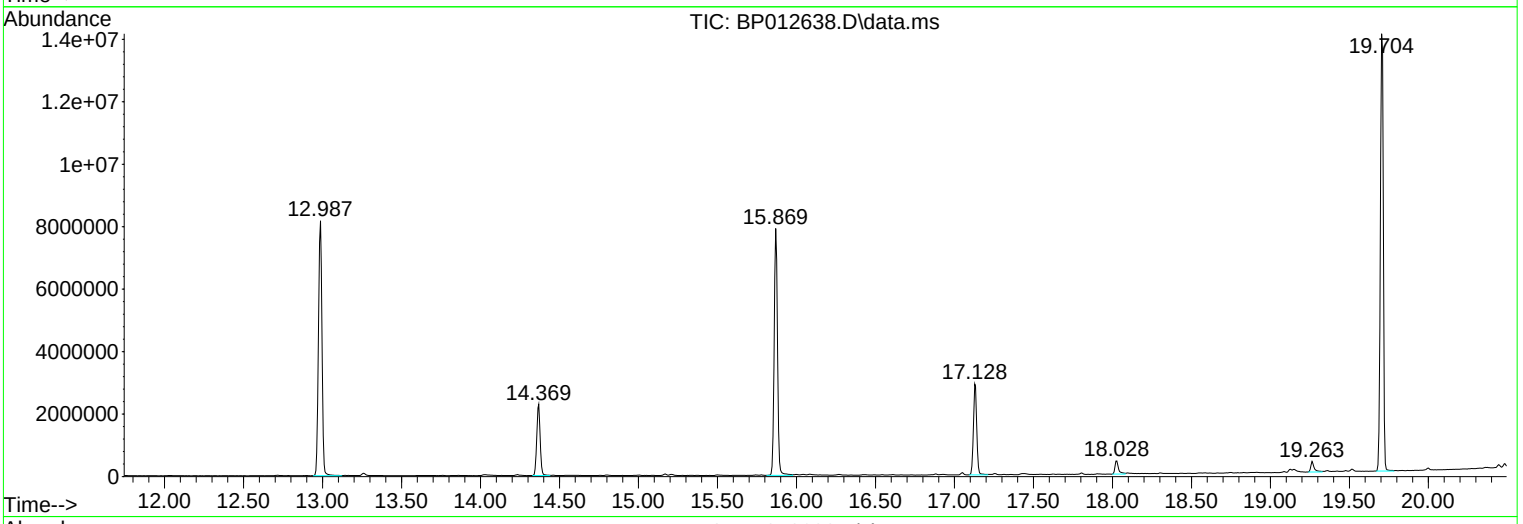
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111222\
Data File : BP012638.D
Acq On : 13 Nov 2022 01:57
Operator : CG/JU
Sample : N5530-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

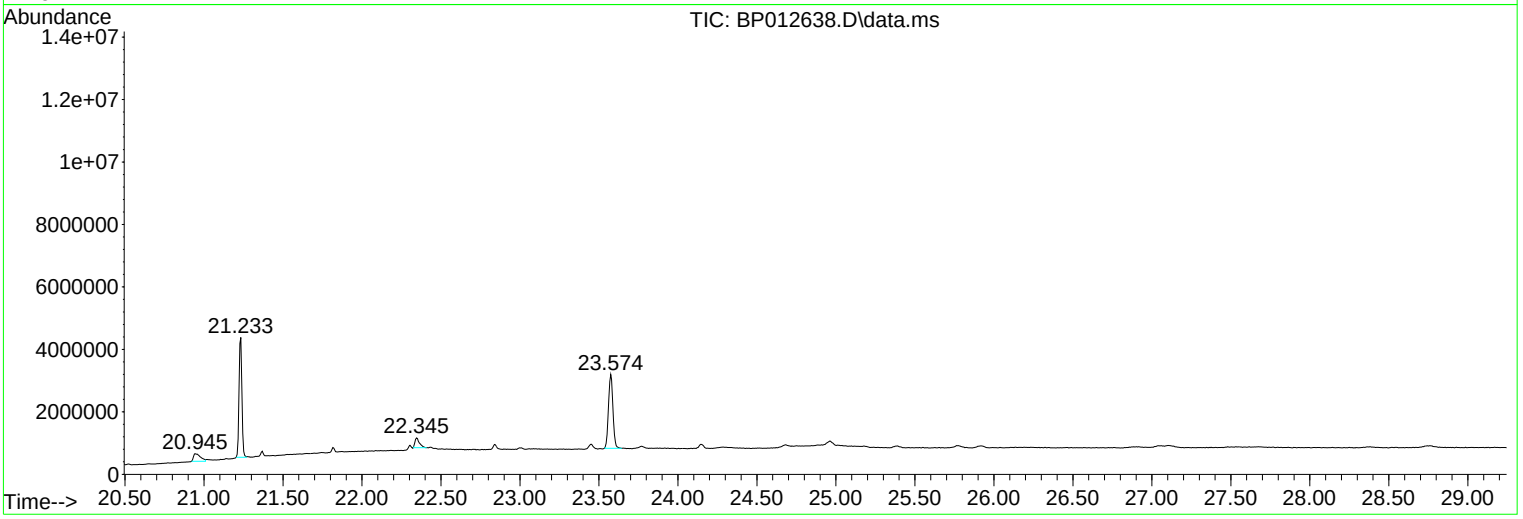
Instrument :
BNA_P
ClientSampleId :
SB-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111222.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\BP111222\
Data File : BP012638.D
Acq On : 13 Nov 2022 01:57
Operator : CG/JU
Sample : N5530-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

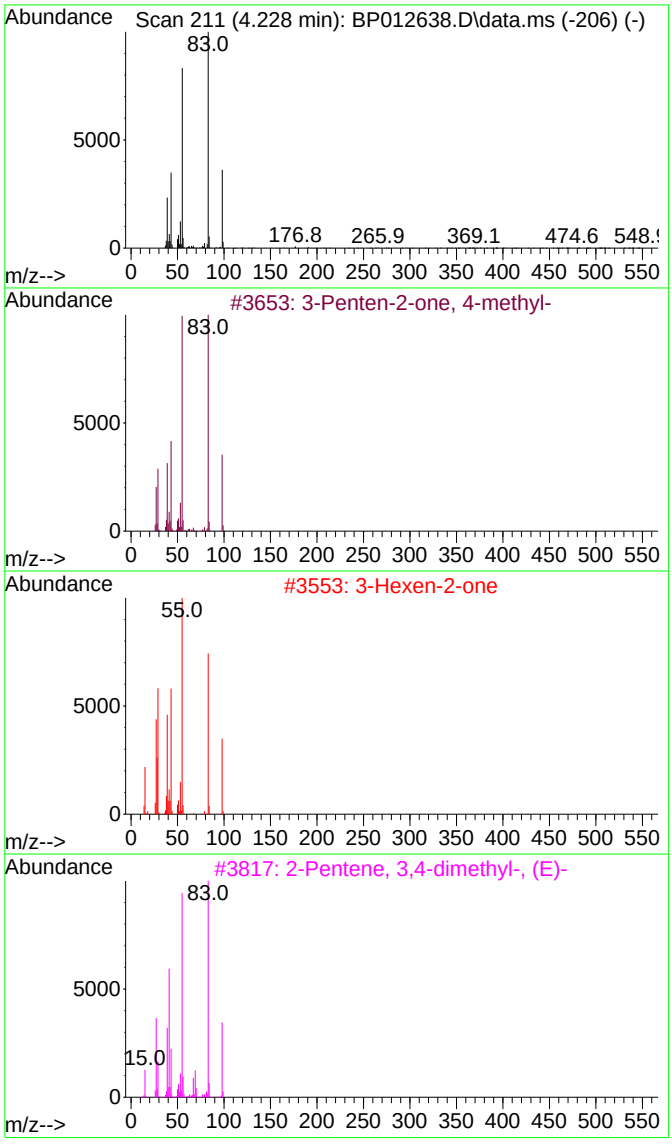
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

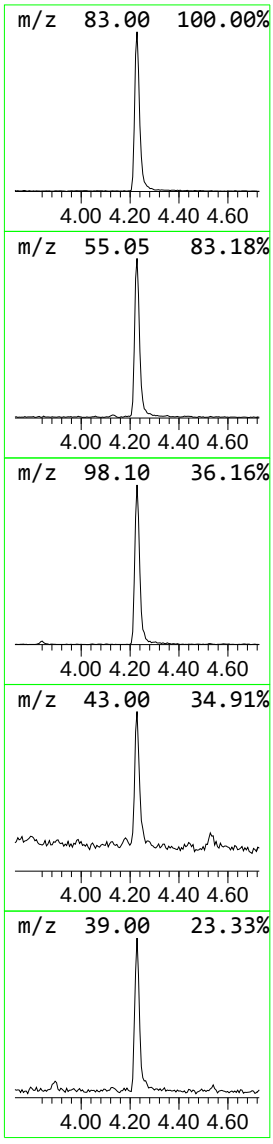
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.228	2.71 ng	219798	1,4-Dichlorobenzene-d4	7.710

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111222\
Data File : BP012638.D
Acq On : 13 Nov 2022 01:57
Operator : CG/JU
Sample : N5530-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-11

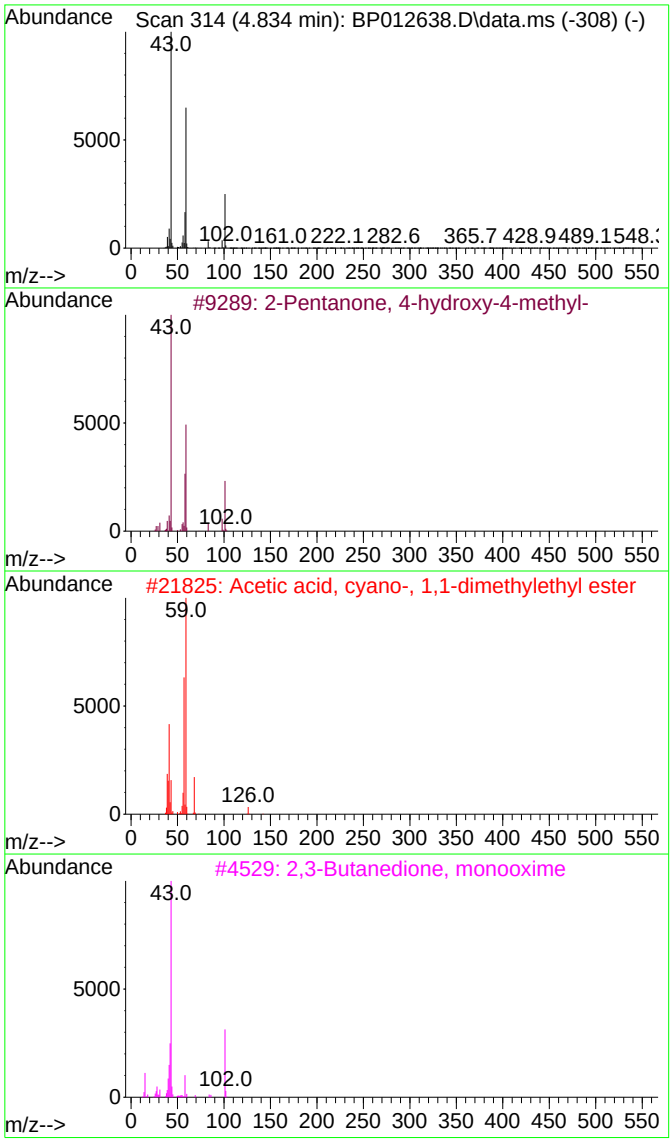
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

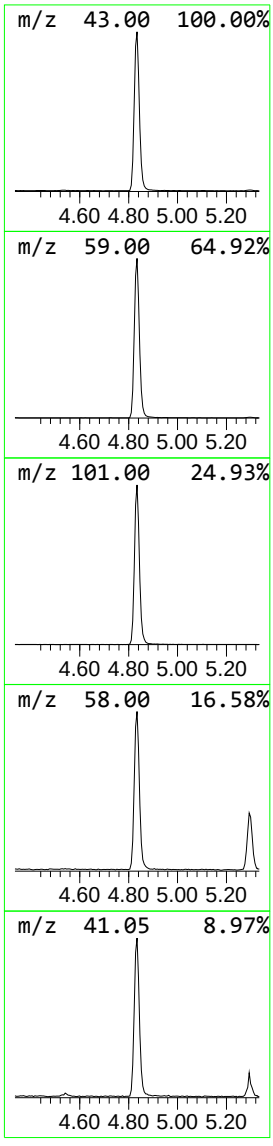
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.834	24.90 ng	2016960	1,4-Dichlorobenzene-d4	7.710

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111222\
Data File : BP012638.D
Acq On : 13 Nov 2022 01:57
Operator : CG/JU
Sample : N5530-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-11

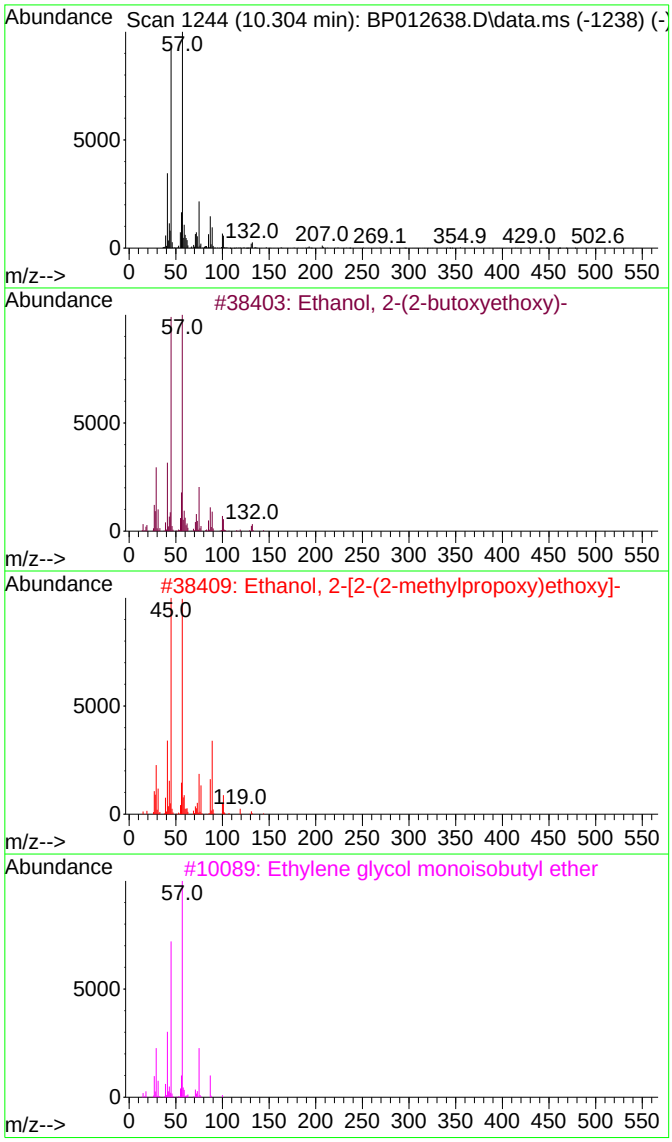
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

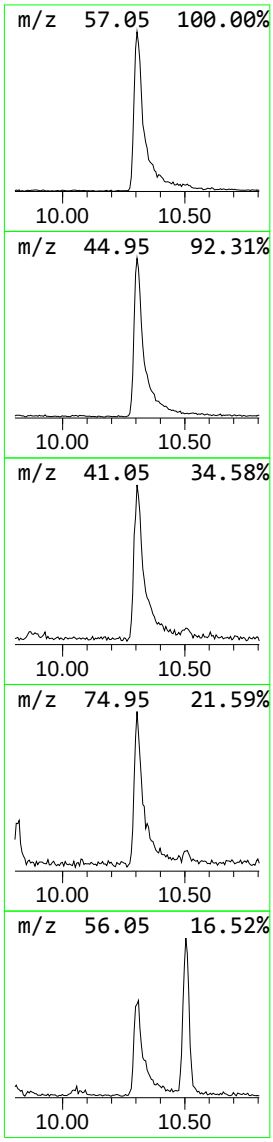
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.305	2.56 ng	305107	Naphthalene-d8	10.505

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	53
5	(2-Ethoxyethoxy)acetic acid, TBD...	262	C12H26O4Si	1000366-92-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111222\
Data File : BP012638.D
Acq On : 13 Nov 2022 01:57
Operator : CG/JU
Sample : N5530-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

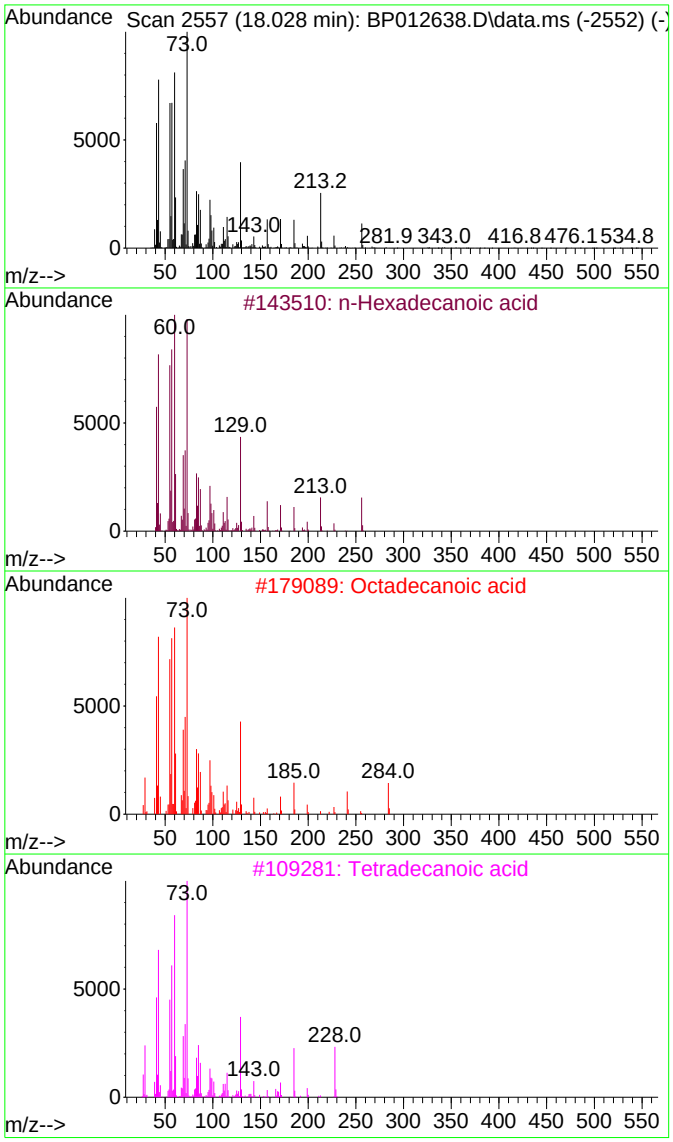
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

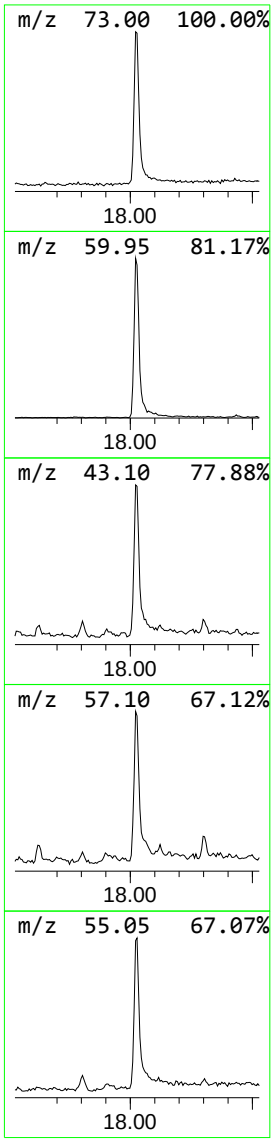
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.028	3.17 ng	673948	Phenanthrene-d10	17.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111222\
Data File : BP012638.D
Acq On : 13 Nov 2022 01:57
Operator : CG/JU
Sample : N5530-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

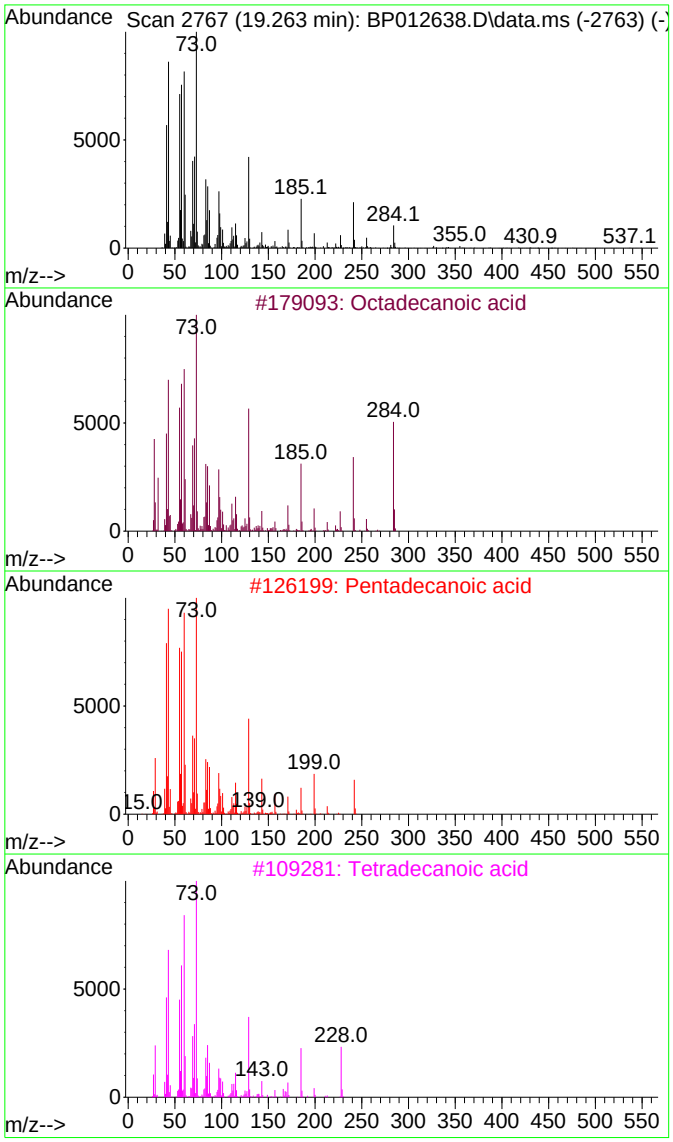
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

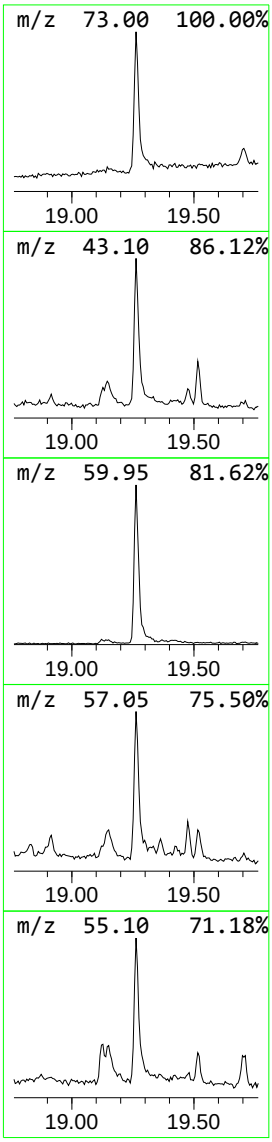
****

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.263	2.12 ng	506333	Chrysene-d12	21.233

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	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111222\
Data File : BP012638.D
Acq On : 13 Nov 2022 01:57
Operator : CG/JU
Sample : N5530-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

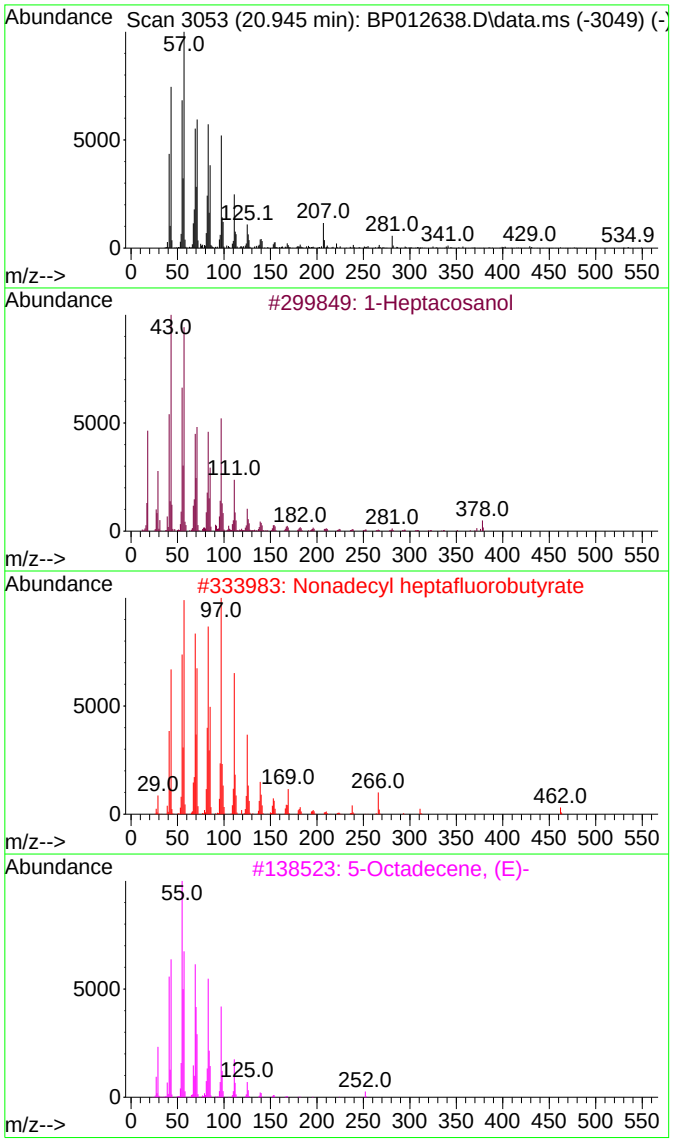
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

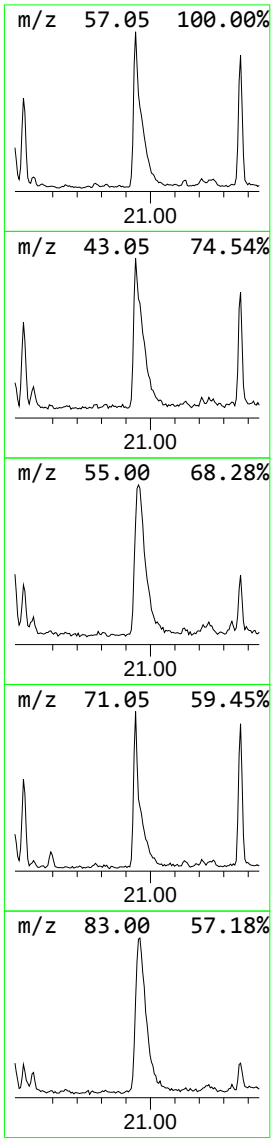
****

Peak Number 6 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.945	3.22 ng	768283	Chrysene-d12	21.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	90
2	Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	90
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	87
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87
5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111222\
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Acq On : 13 Nov 2022 01:57
Operator : CG/JU
Sample : N5530-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-11

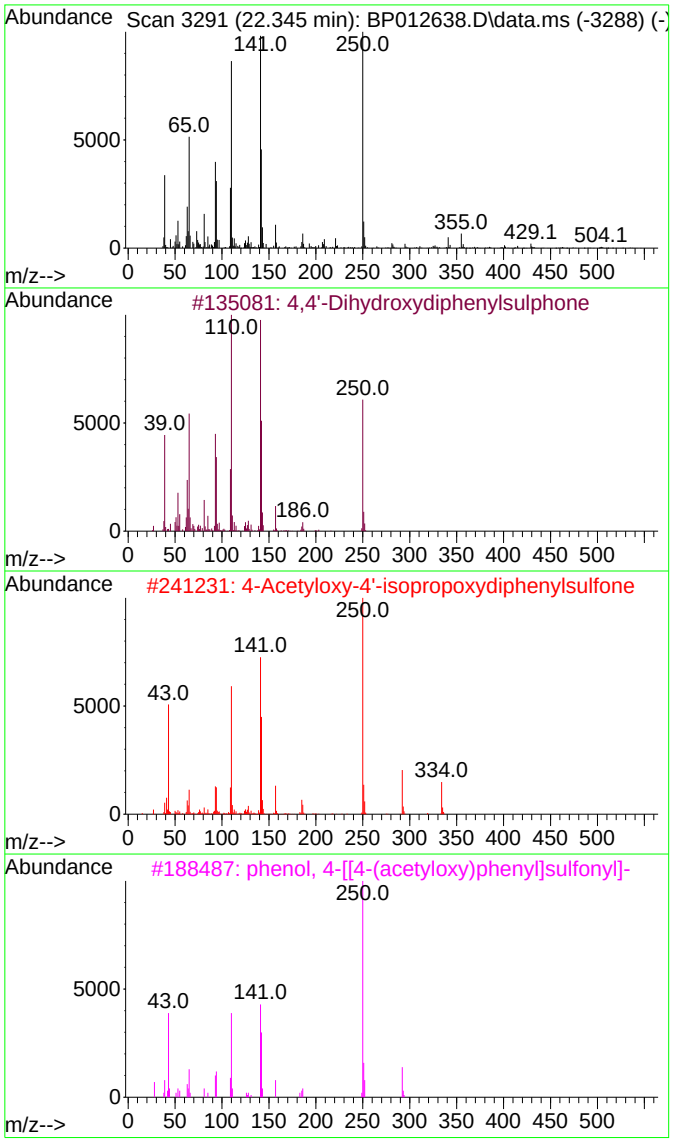
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

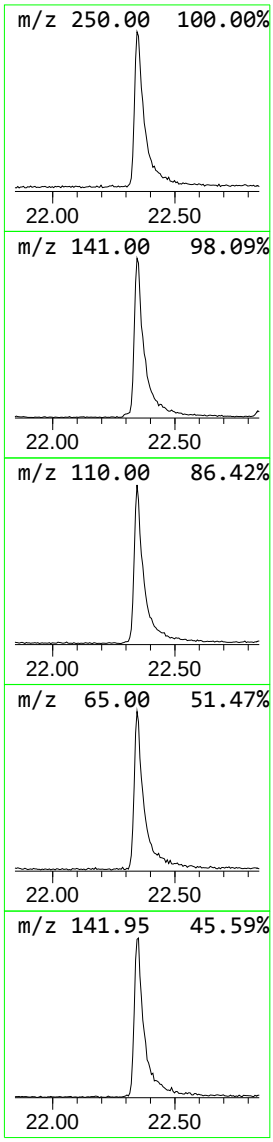
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4,4'-Dihydroxydiphenylsulphone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.345	2.51 ng	600768	Chrysene-d12	21.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	96
2	4-Acetyloxy-4'-isopropoxydipheny...	334	C17H18O5S	158442-42-3	35
3	phenol, 4-[[4-(acetyloxy)phenyl]...	292	C14H12O5S	1000402-05-8	32
4	3,3'-Dihydroxyazoxybenzene	230	C12H10N2O3	017540-51-1	12
5	1-[5-Nitro-6-uracilyl]-2-[2-chlo...	293	C12H8ClN3O4	296798-53-3	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111222\
Data File : BP012638.D
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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
3-Penten-2-one,...	4.228	2.7	ng	219798	1	7.710	1619970	20.0
2-Pentanone, 4-...	4.834	24.9	ng	2016960	1	7.710	1619970	20.0
Ethanol, 2-(2-b...	10.305	2.6	ng	305107	2	10.505	2387280	20.0
n-Hexadecanoic ...	18.028	3.2	ng	673948	4	17.128	4248610	20.0
Octadecanoic acid	19.263	2.1	ng	506333	5	21.233	4779290	20.0
1-Heptacosanol	20.945	3.2	ng	768283	5	21.233	4779290	20.0
4,4'-Dihydroxyd...	22.345	2.5	ng	600768	5	21.233	4779290	20.0