LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

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-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008287.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.299	219	223	230	rBV	113973	150707	3.36%	0.602%
2	4.899	319	325	337	rBV	538715	738980	16.49%	2.950%
3	5.369	398	405	418	rBV	1514871	2292899	51.15%	9.154%
4	6.963	667	676	692	rBV	1388942	2355785	52.55%	9.405%
5	7.769	804	813	822	rBV	315838	485248	10.83%	1.937%
6	8.934	1003	1011	1027	rBV	898736	1523972	34.00%	6.084%
7	10.363	1247	1254	1275	rBV	212633	508283	11.34%	2.029%
8	10.569	1281	1289	1305	rVB	378805	644707	14.38%	2.574%
9	13.045	1701	1710	1724	rBV	2105465	3223006	71.90%	12.867%
10	13.334	1752	1759	1768	rBV	152806	263683	5.88%	1.053%
11	14.422	1938	1944	1960	rVB	572452	883462	19.71%	3.527%
12	15.422	2109	2114	2128	rVB3	27503	57522	1.28%	0.230%
13	15.928	2189	2200	2223	rBV	1779160	2666273	59.48%	10.644%
14	17.186	2408	2414	2426	rBV	711585	1069711	23.86%	4.271%
15	17.869	2526	2530	2538	rVB	51953	70998	1.58%	0.283%
16	18.092	2563	2568	2576	rBV	141316	214949	4.80%	0.858%
17	18.927	2706	2710	2716	rBV2	36141	58017	1.29%	0.232%
18	19.010	2720	2724	2728	rVB	149684	172161	3.84%	0.687%
19	19.139	2742	2746	2749	rVB	60931	64417	1.44%	0.257%
20	19.269	2764	2768	2771	rVB	42321	45993	1.03%	0.184%
21	19.763	2847	2852	2862	rBV	3669082	4482596	100.00%	17.896%
22	20.045	2896	2900	2907	rBV	115680	183407	4.09%	0.732%
23	20.392	2955	2959	2963	rVB	142793	165100	3.68%	0.659%
24	20.445	2965	2968	2974	rVB2	44665	58685	1.31%	0.234%
25	20.516	2976	2980	2983	rVV	66592	69609	1.55%	0.278%
26	21.016	3061	3065	3072	rBV2	206958	305532	6.82%	1.220%
27	21.080	3073	3076	3080	rVB	79695	91125	2.03%	0.364%
28	21.210	3095	3098	3105	rBV	59901	63269	1.41%	0.253%
29	21.298	3108	3113	3118	rBV	778286	1016667	22.68%	4.059%
30	21.386	3126	3128	3131	rBV	46922	50036	1.12%	0.200%
31	22.539	3321	3324	3329	rVB	149188	212161	4.73%	0.847%
32	23.692	3514	3520	3528	rVB	415435	859546	19.18%	3.432%

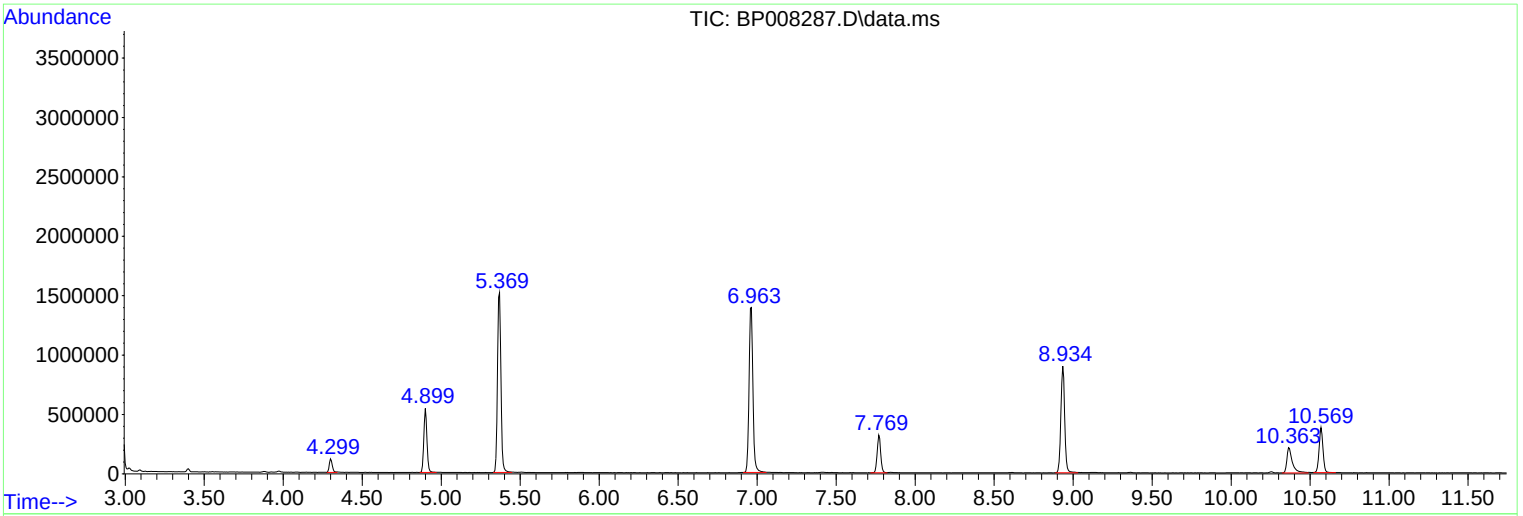
Sum of corrected areas: 25048506

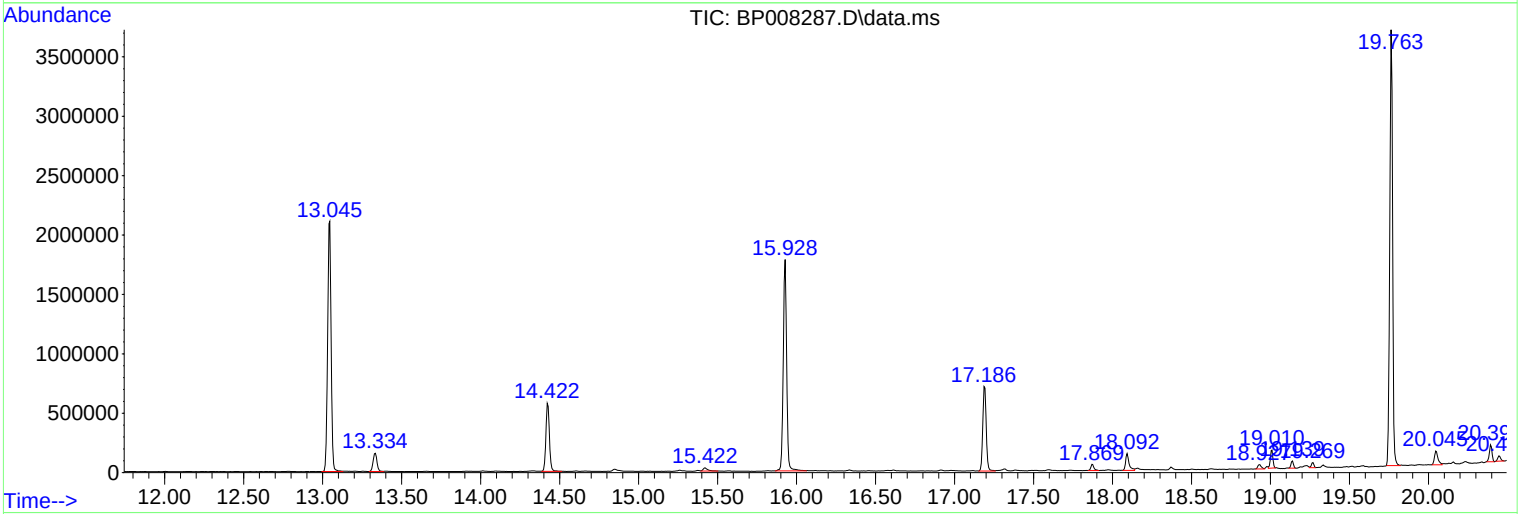
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

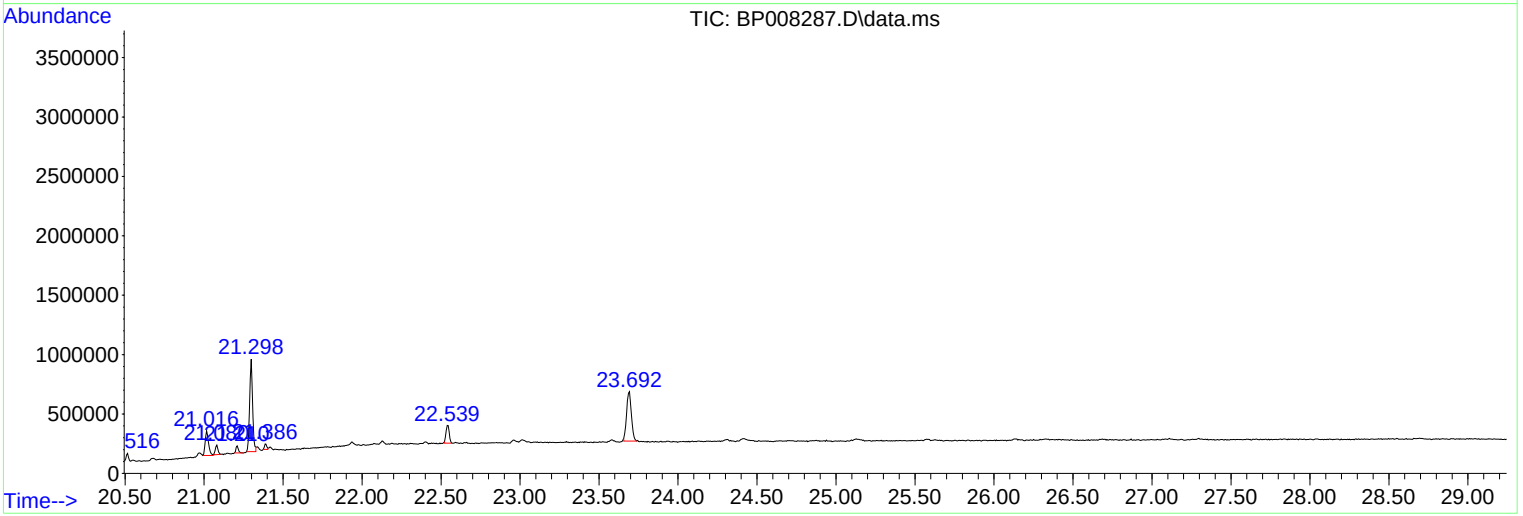
Instrument :
BNA_P
ClientSampleId :
TP-5S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

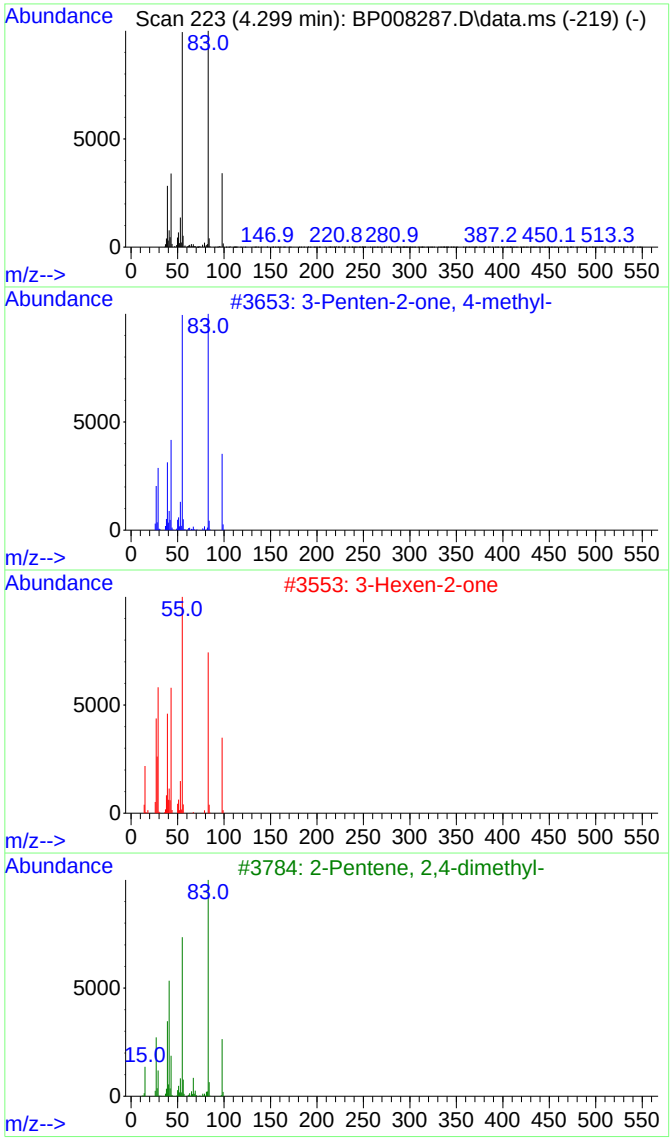
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

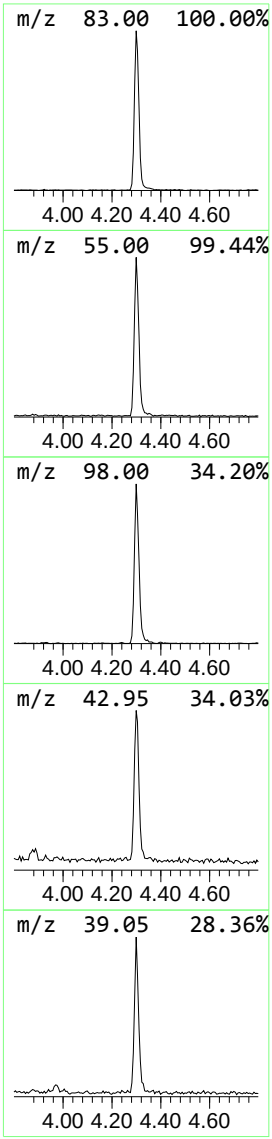
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.299	6.21 ng	150707	1,4-Dichlorobenzene-d4	7.769

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, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

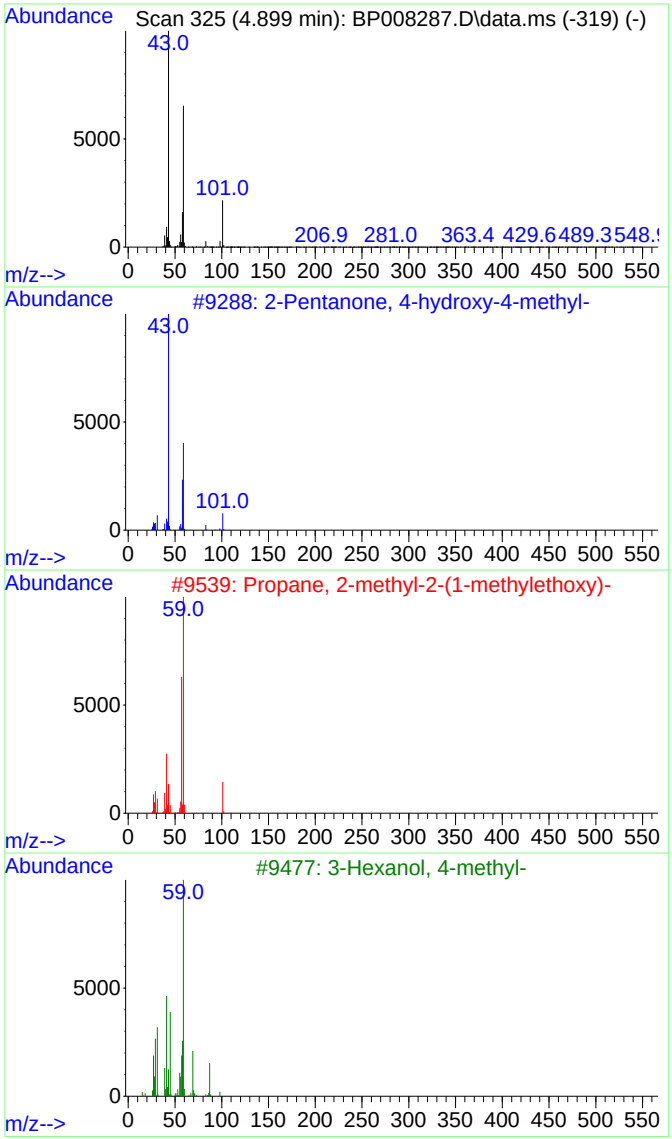
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

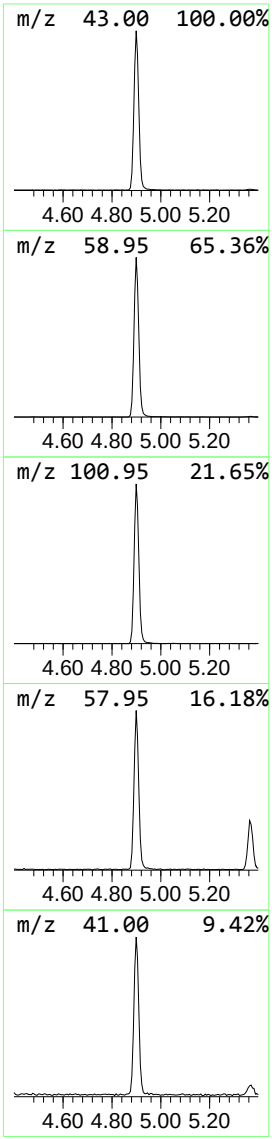
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.899	30.46 ng	738980	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

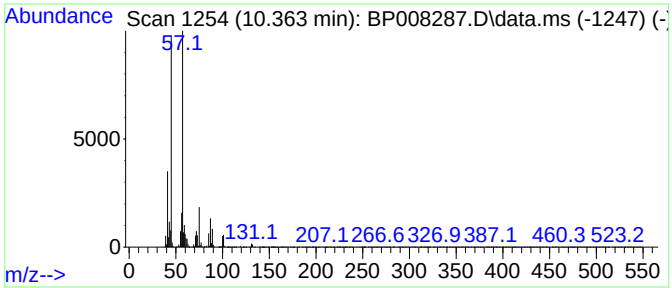
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

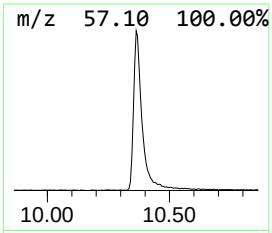
****

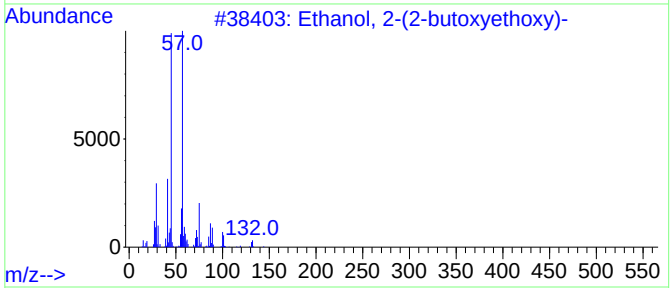
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

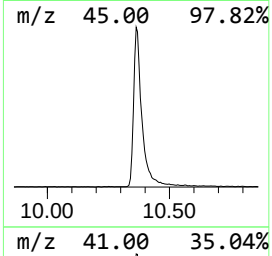
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.363	15.77 ng	508283	Naphthalene-d8	10.569

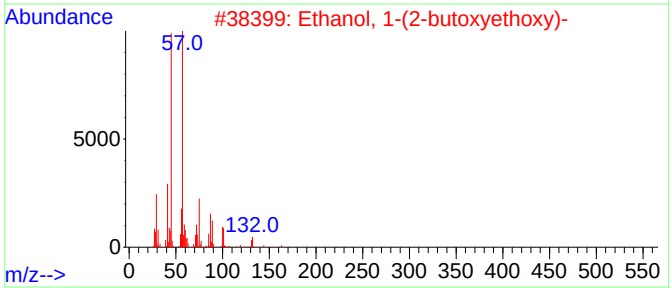
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	59
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56

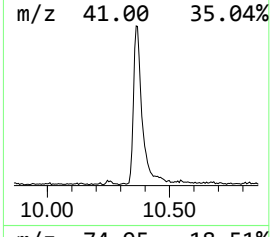


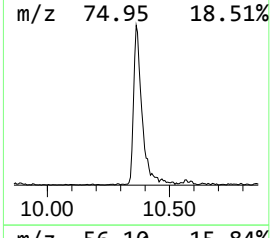


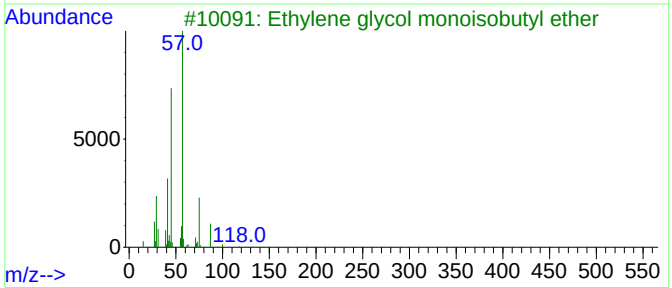


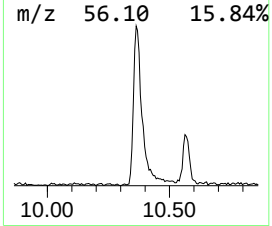












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

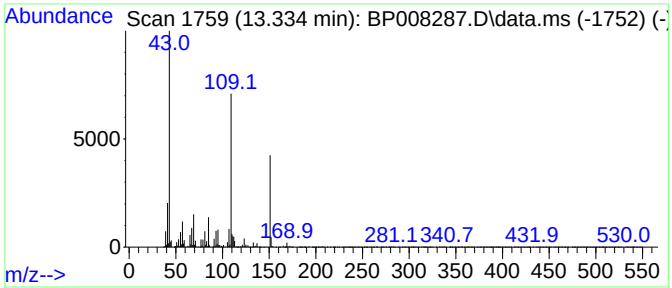
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

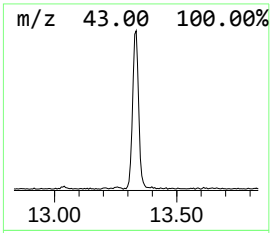
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

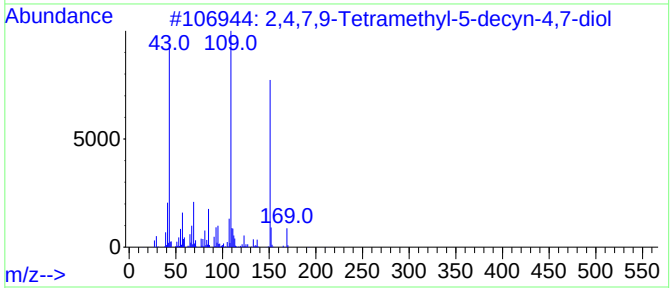
****
Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

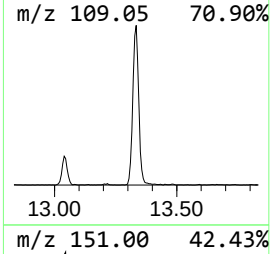
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.334	5.97 ng	263683	Acenaphthene-d10	14.422

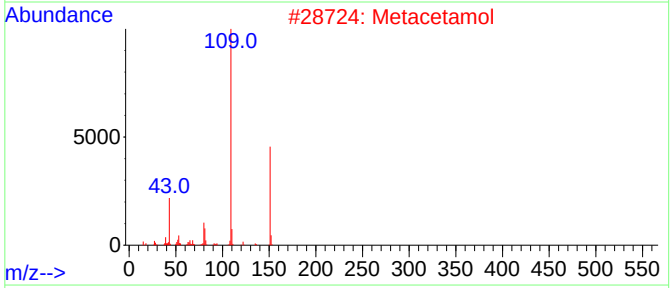
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	58
3	Acetaminophen	151	C8H9NO2	000103-90-2	53
4	N-(4-tert-Butoxyphenyl)acetamide...	249	C14H19NO3	1000504-17-4	53
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53

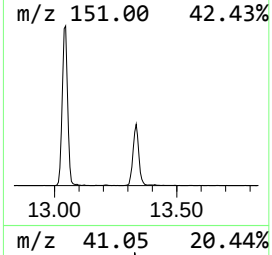


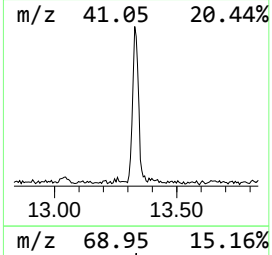


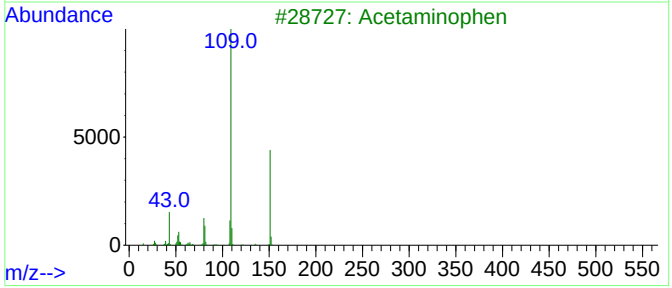


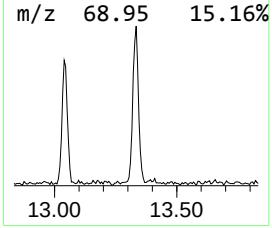












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

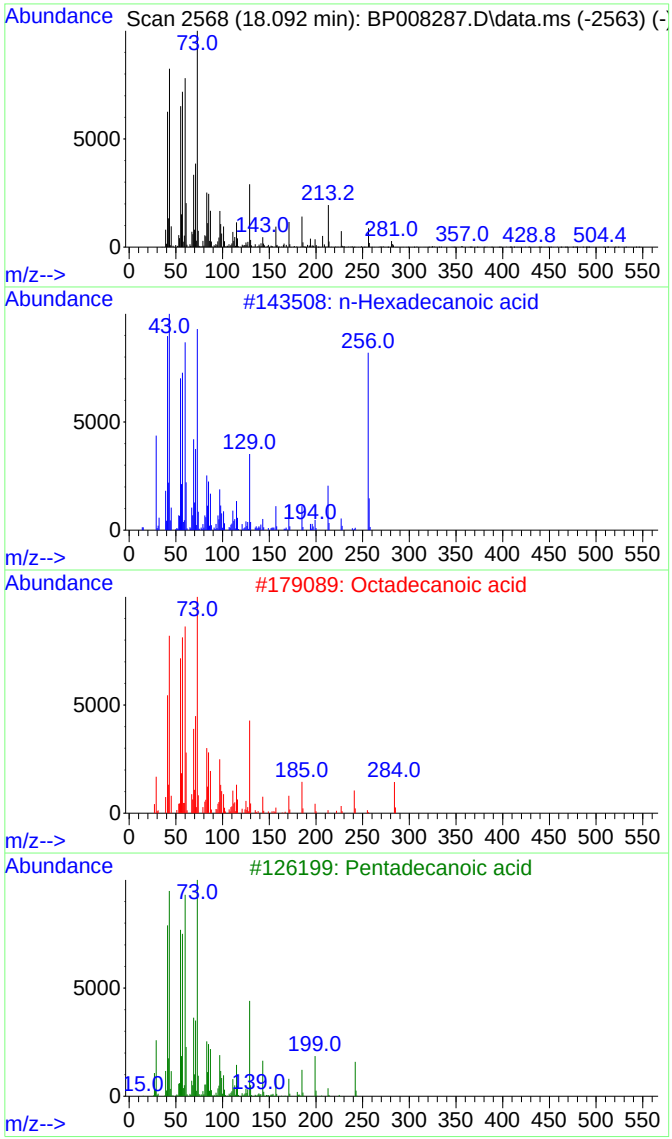
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

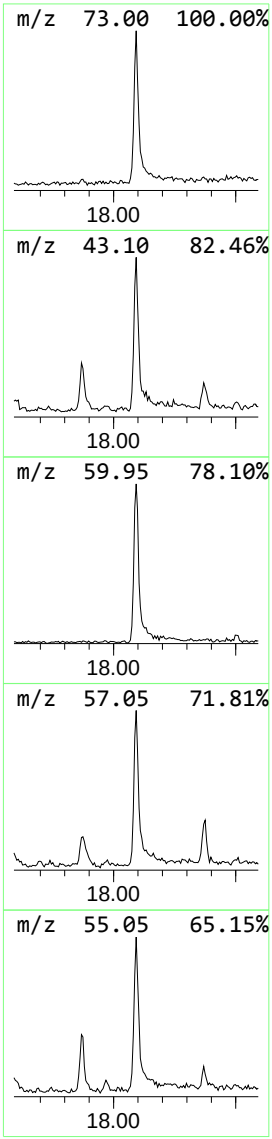
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	4.02 ng	214949	Phenanthrene-d10	17.186

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	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

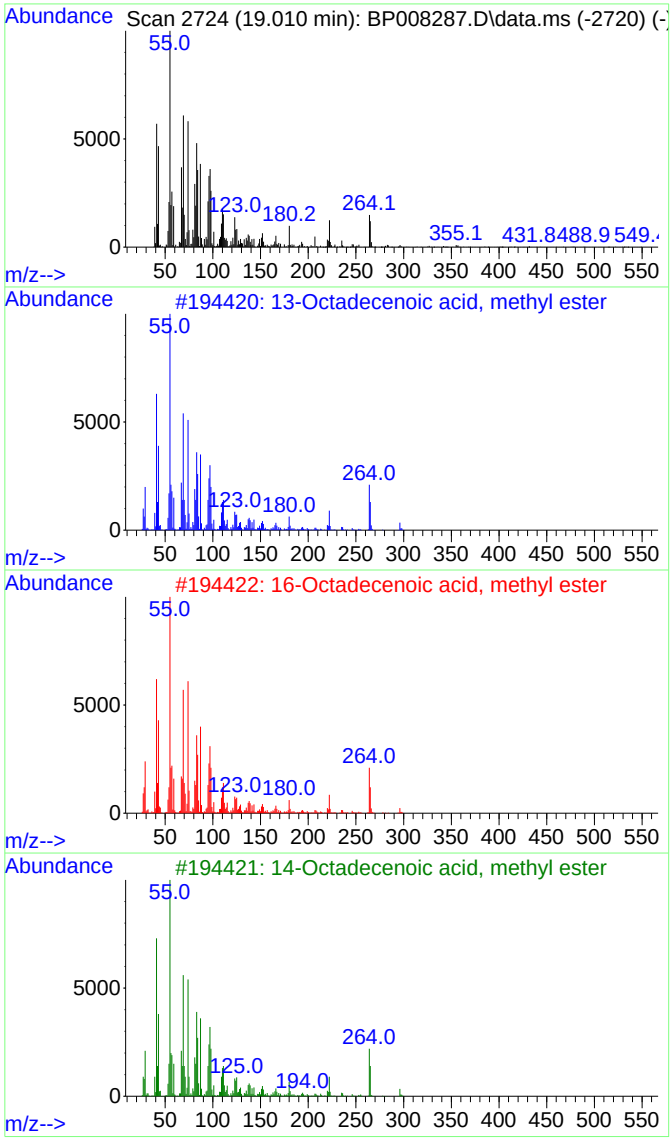
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

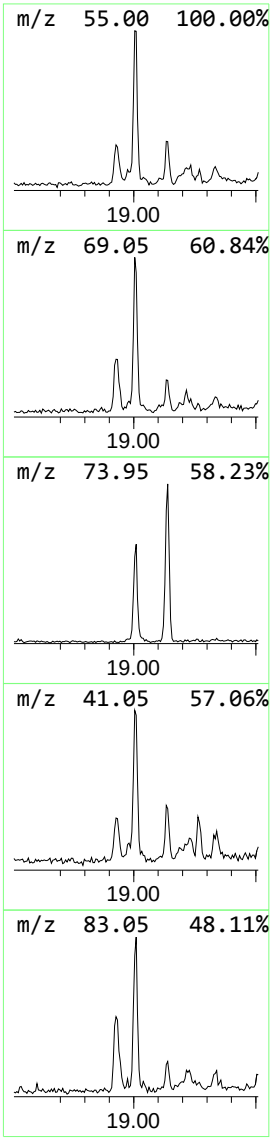
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 13-Octadecenoic acid, methy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.010	3.22 ng	172161	Phenanthrene-d10	17.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	97
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	95
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	94
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

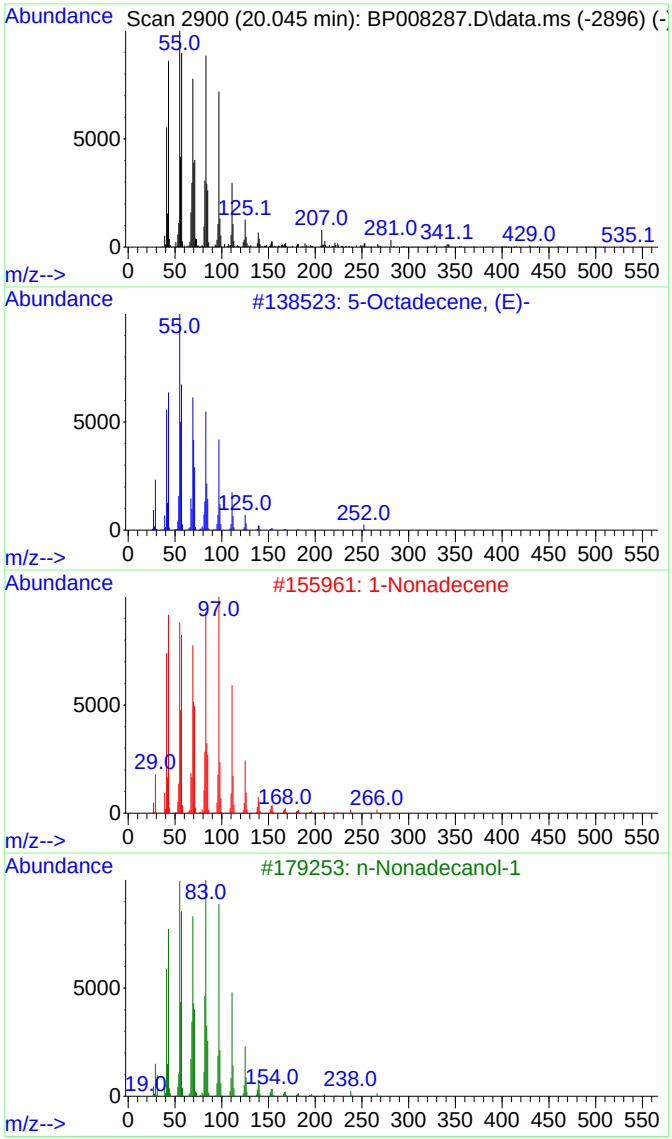
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

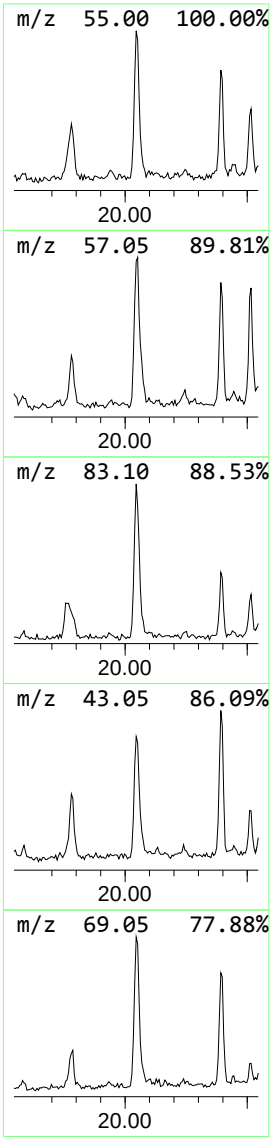
****

Peak Number 7 5-Octadecene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.045	3.61 ng	183407	Chrysene-d12	21.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	1-Octadecanol	270	C18H38O	000112-92-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

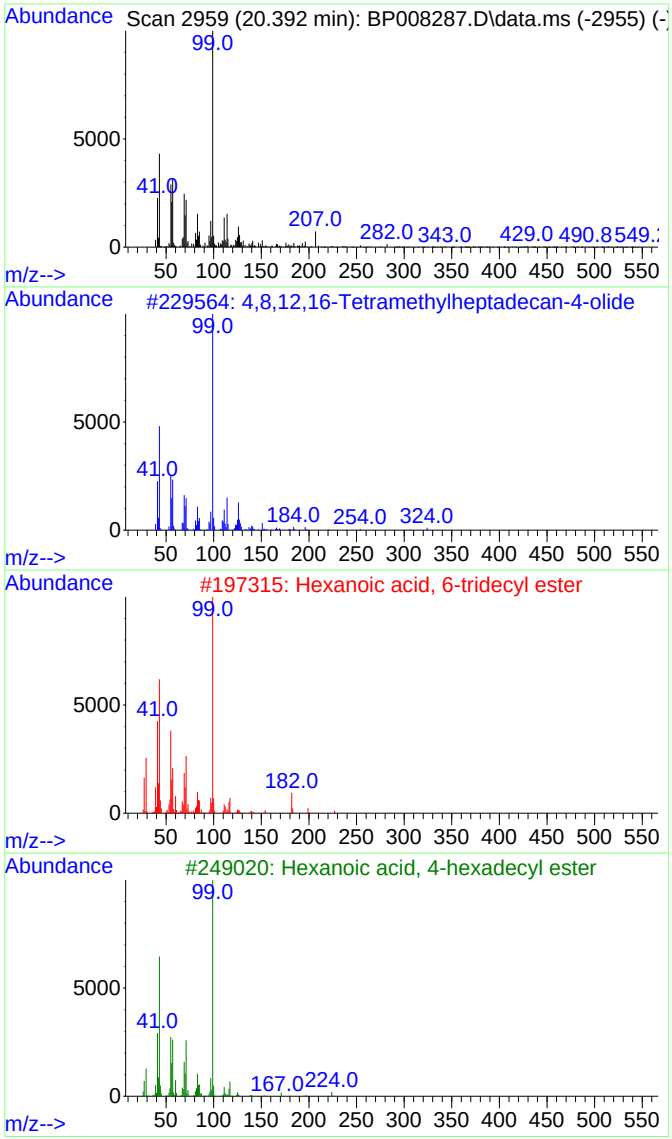
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

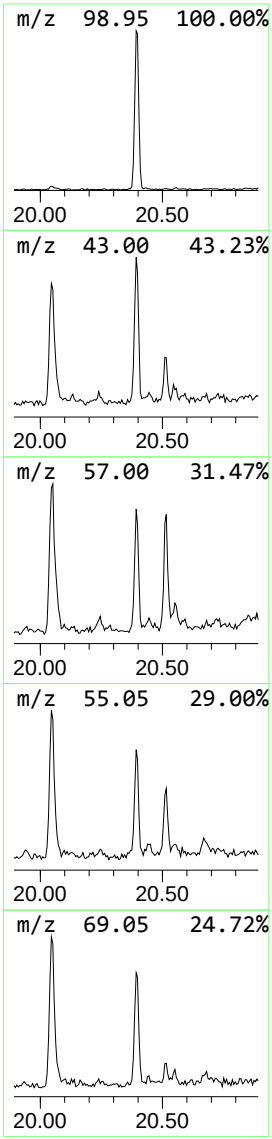
****

Peak Number 8 4,8,12,16-Tetramethylheptad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.392	3.25 ng	165100	Chrysene-d12	21.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	74
2	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	53
3	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	53
4	Esaprazole	225	C12H23N3O	064204-55-3	49
5	Pyrimidine-2,4,6-trione, 1-butyl...	323	C15H25N5O3	1000304-28-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

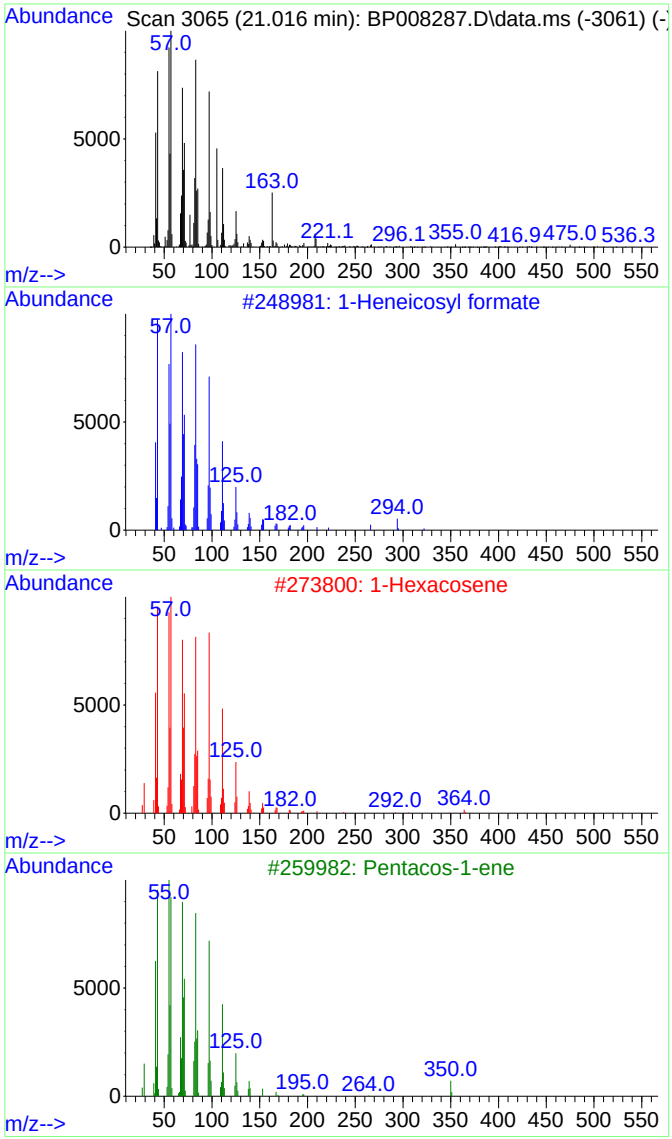
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

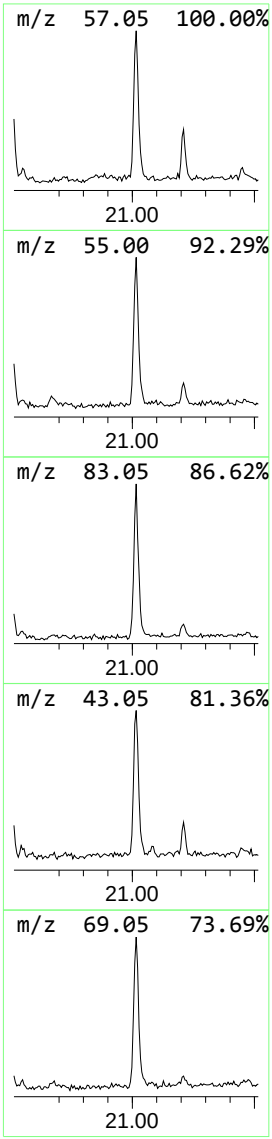
****

Peak Number 9 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.016	6.01 ng	305532	Chrysene-d12	21.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	Pentacos-1-ene	350	C25H50	016980-85-1	93
4	Heptacos-1-ene	378	C27H54	015306-27-1	93
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

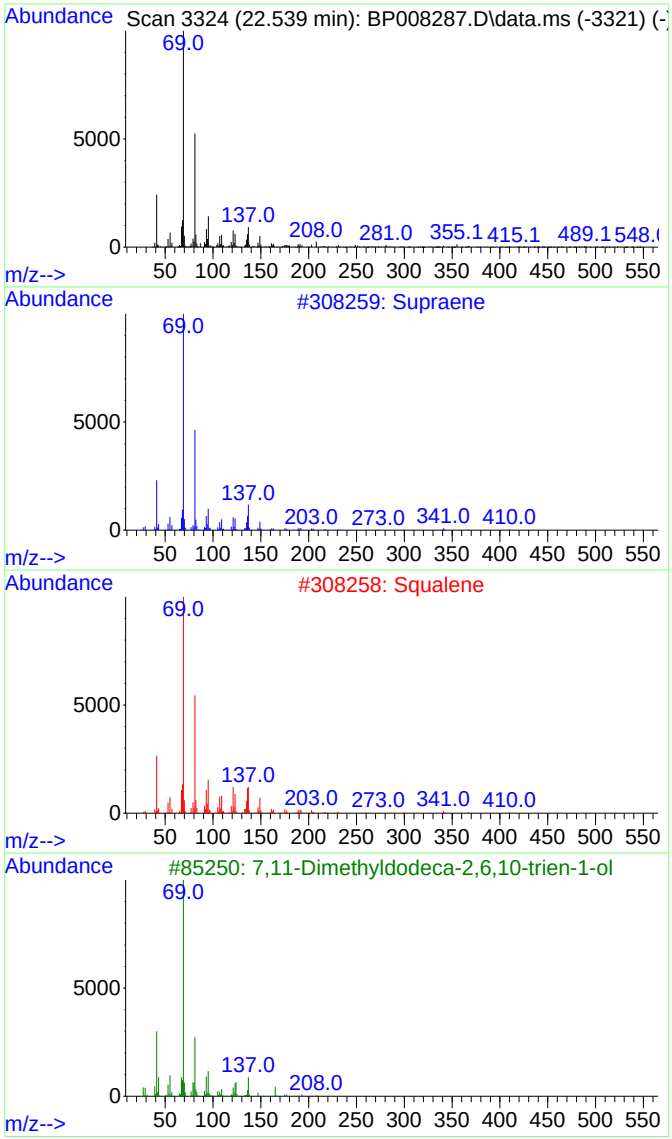
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

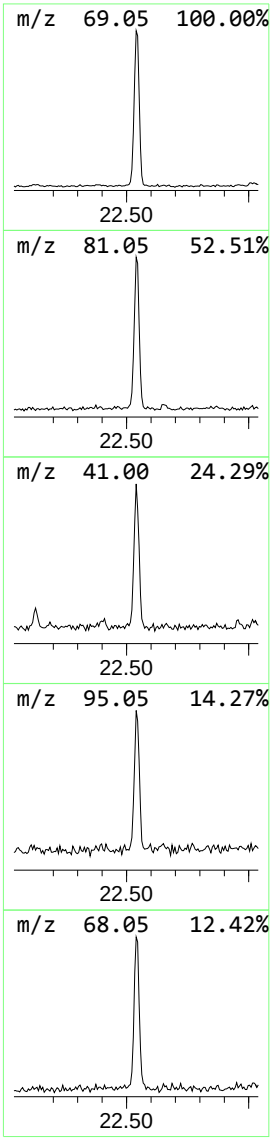
****

Peak Number 10 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.539	4.94 ng	212161	Perylene-d12	23.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	98
2	Squalene	410	C30H50	000111-02-4	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008287.D
Acq On : 08 Dec 2021 19:50
Operator : CG/JU
Sample : M4959-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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
3-Penten-2-one,...	4.299	6.2	ng	150707	1	7.769	485248	20.0
2-Pentanone, 4-...	4.899	30.5	ng	738980	1	7.769	485248	20.0
Ethanol, 2-(2-b...	10.363	15.8	ng	508283	2	10.569	644707	20.0
2,4,7,9-Tetrame...	13.334	6.0	ng	263683	3	14.422	883462	20.0
n-Hexadecanoic ...	18.092	4.0	ng	214949	4	17.186	1069710	20.0
13-Octadecenoic...	19.010	3.2	ng	172161	4	17.186	1069710	20.0
5-Octadecene, (E)-	20.045	3.6	ng	183407	5	21.298	1016670	20.0
4,8,12,16-Tetra...	20.392	3.3	ng	165100	5	21.298	1016670	20.0
1-Heneicosyl fo...	21.016	6.0	ng	305532	5	21.298	1016670	20.0
Supraene	22.539	4.9	ng	212161	6	23.692	859546	20.0