LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006545.D
Acq On : 06 Aug 2021 18:47
Operator : CG/JU
Sample : M3279-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20210532-COM-5

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-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006545.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.905	304	309	319	rVB	1479160	2004232	27.28%	4.218%
2	5.358	380	386	396	rVB	3881139	5367629	73.06%	11.297%
3	5.970	485	490	500	rVB	298032	438941	5.97%	0.924%
4	6.934	647	654	666	rBV	3556727	5423946	73.83%	11.416%
5	7.752	787	793	800	rBV	726981	1144636	15.58%	2.409%
6	8.911	982	990	999	rBV	2176949	3456404	47.04%	7.275%
7	10.328	1225	1231	1246	rBV	328822	546899	7.44%	1.151%
8	10.534	1258	1266	1280	rVB	914200	1552690	21.13%	3.268%
9	13.010	1678	1687	1698	rBV	4035927	5981374	81.41%	12.589%
10	14.381	1911	1920	1928	rBV	1206155	1743662	23.73%	3.670%
11	15.875	2164	2174	2205	rBV	3192355	4644953	63.22%	9.776%
12	17.134	2382	2388	2397	rBV	1325446	1901757	25.88%	4.003%
13	18.040	2537	2542	2551	rBV	352360	578611	7.88%	1.218%
14	19.281	2749	2753	2767	rBV	339469	599262	8.16%	1.261%
15	19.710	2821	2826	2832	rBV	6348085	7347028	100.00%	15.464%
16	20.957	3035	3038	3044	rBV	288457	356309	4.85%	0.750%
17	21.233	3080	3085	3090	rBV	1677693	2097505	28.55%	4.415%
18	23.557	3474	3480	3488	rBV2	1179517	2326197	31.66%	4.896%

Sum of corrected areas: 47512035

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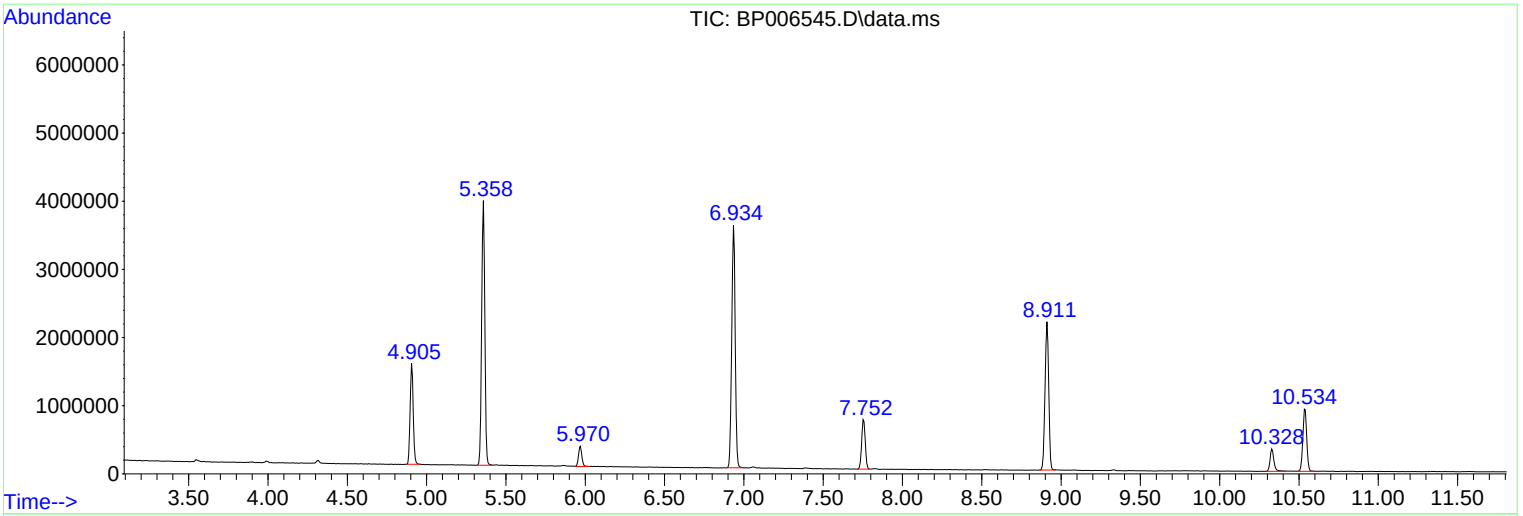
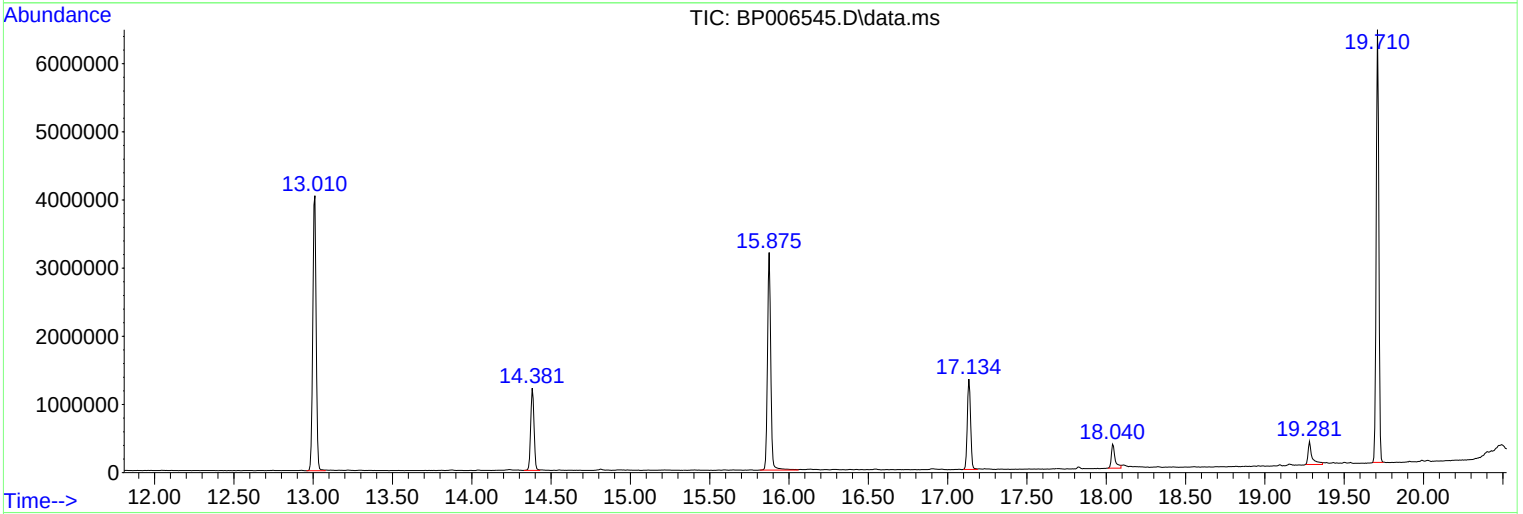
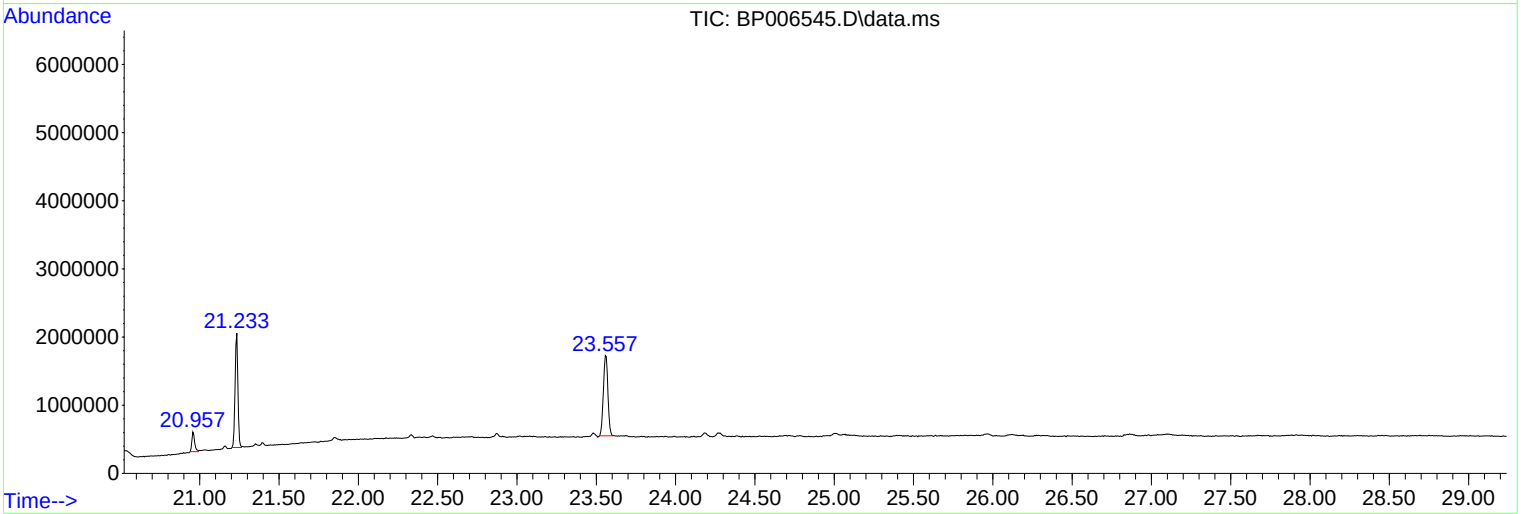
Instrument :
BNA_P
ClientSampleId :
20210532-COM-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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Sample : M3279-11
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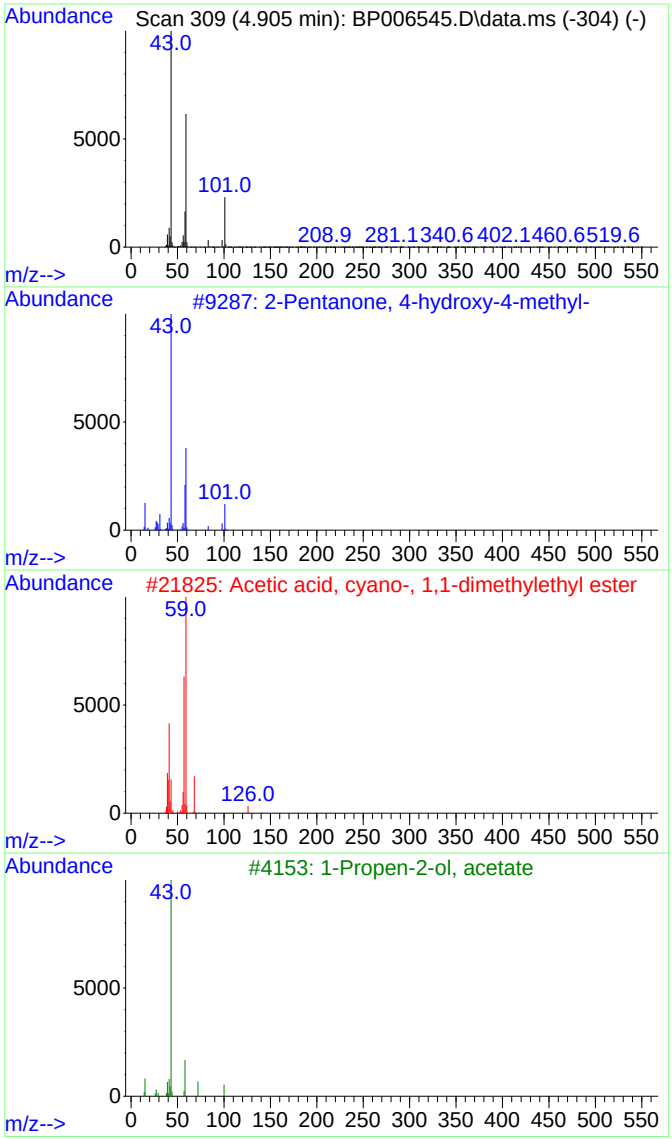
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

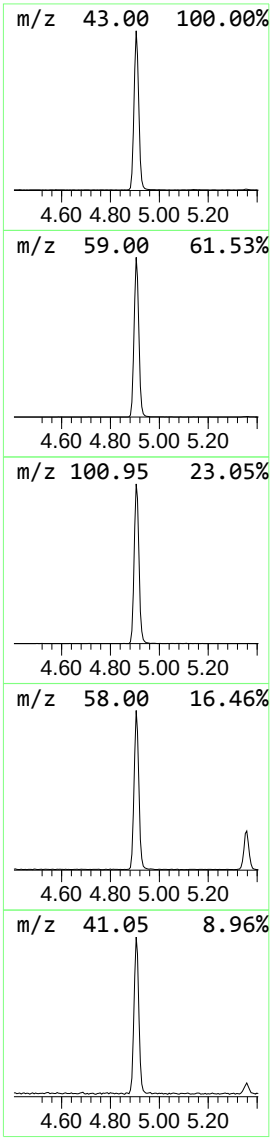
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	35.02 ng	2004230	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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ClientSampleId :
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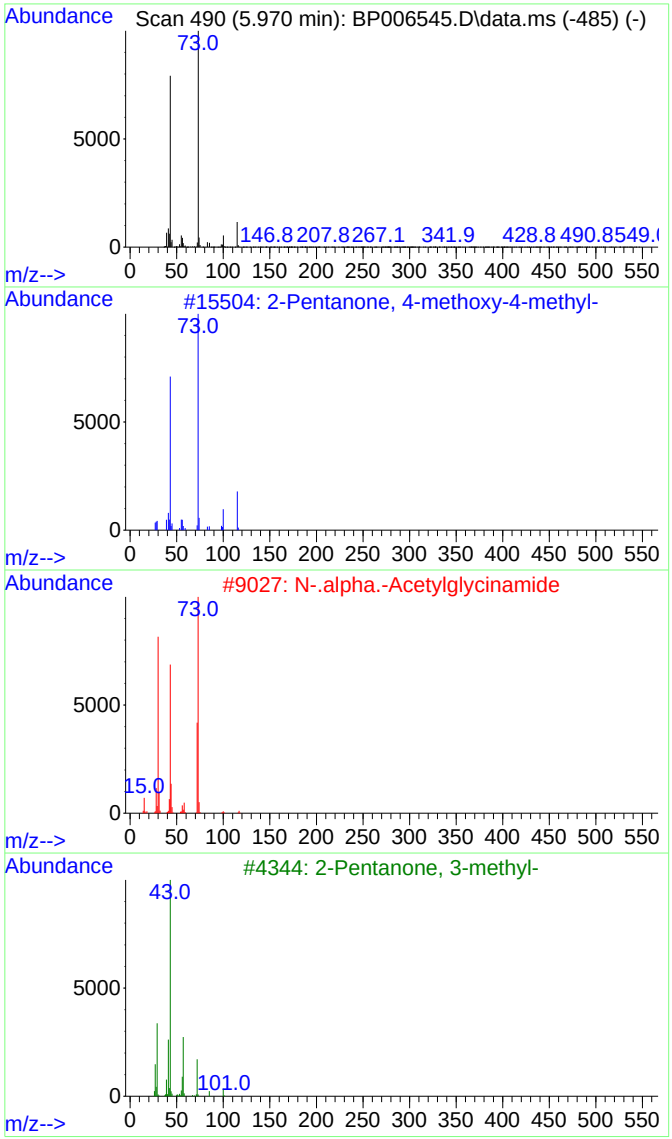
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

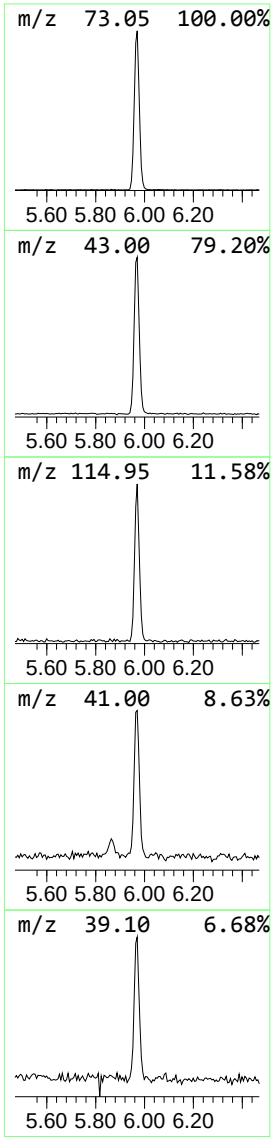
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.970	7.67 ng	438941	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10





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Operator : CG/JU
Sample : M3279-11
Misc :
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Instrument :
BNA_P
ClientSampleId :
20210532-COM-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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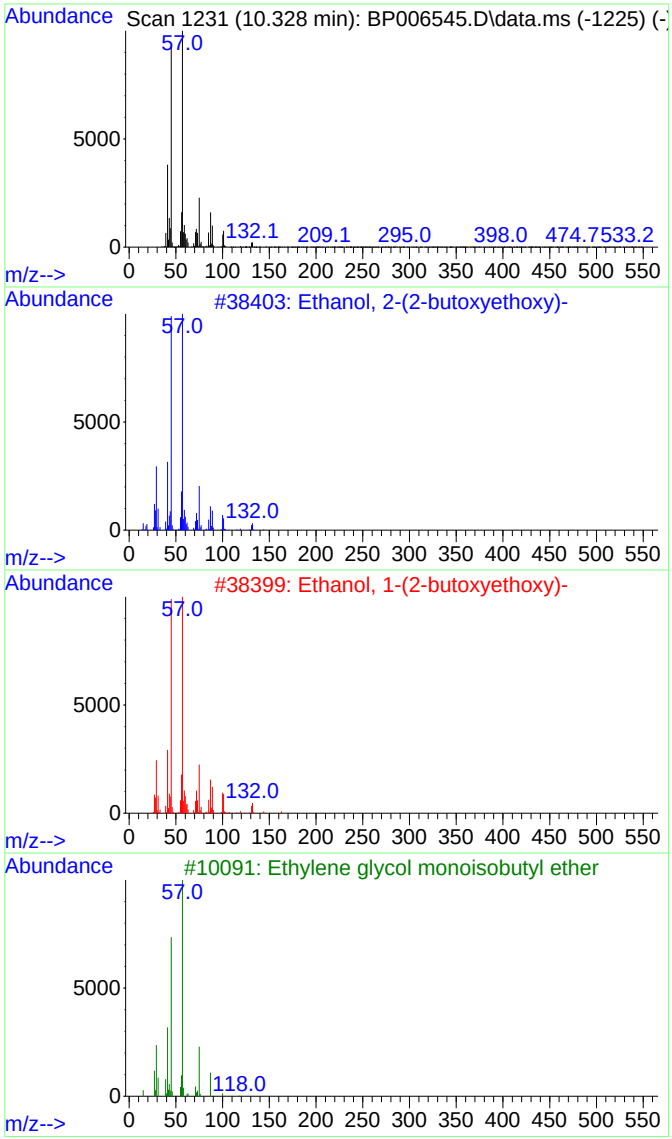
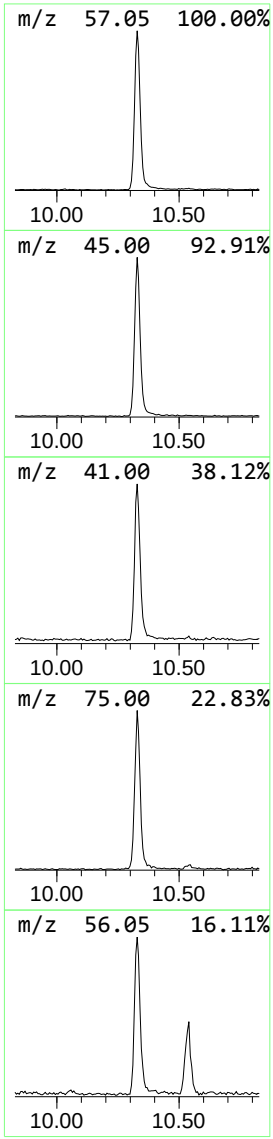
****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	7.04 ng	546899	Naphthalene-d8	10.534

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	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52





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BNA_P
ClientSampleId :
20210532-COM-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
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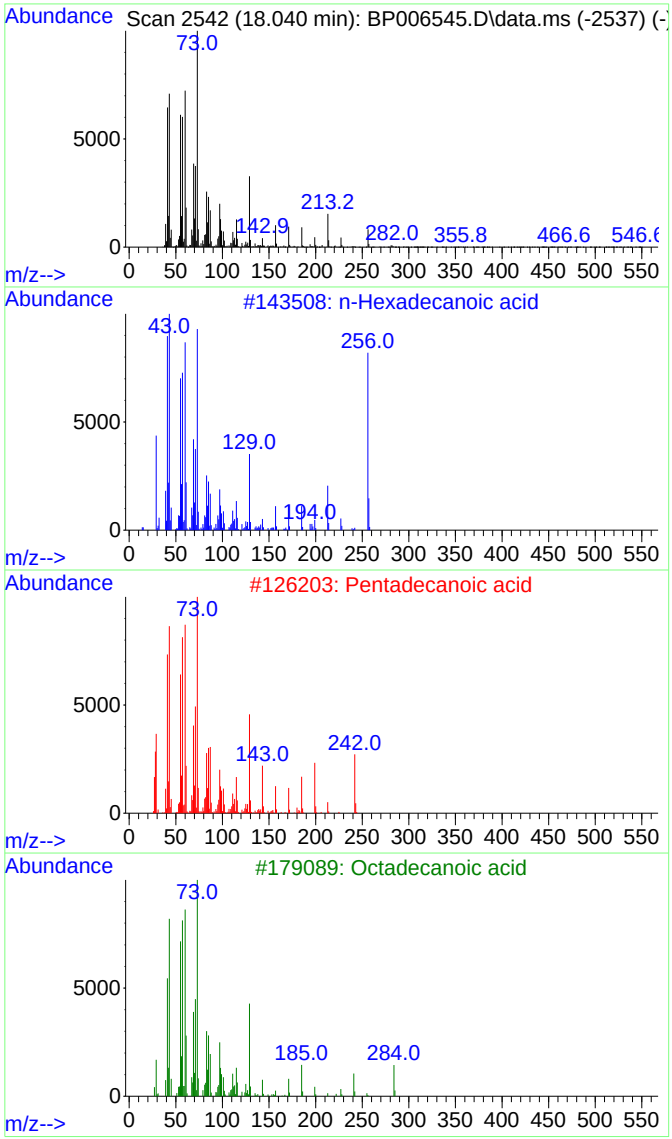
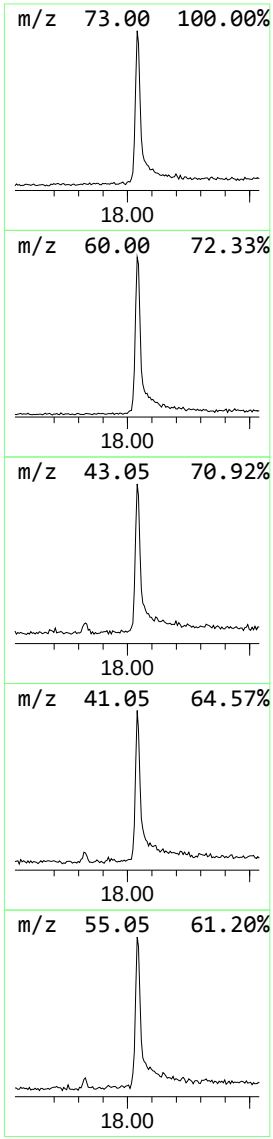
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.040	6.09 ng	578611	Phenanthrene-d10	17.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Octadecanoic acid	284	C18H36O2	000057-11-4	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





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Sample : M3279-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20210532-COM-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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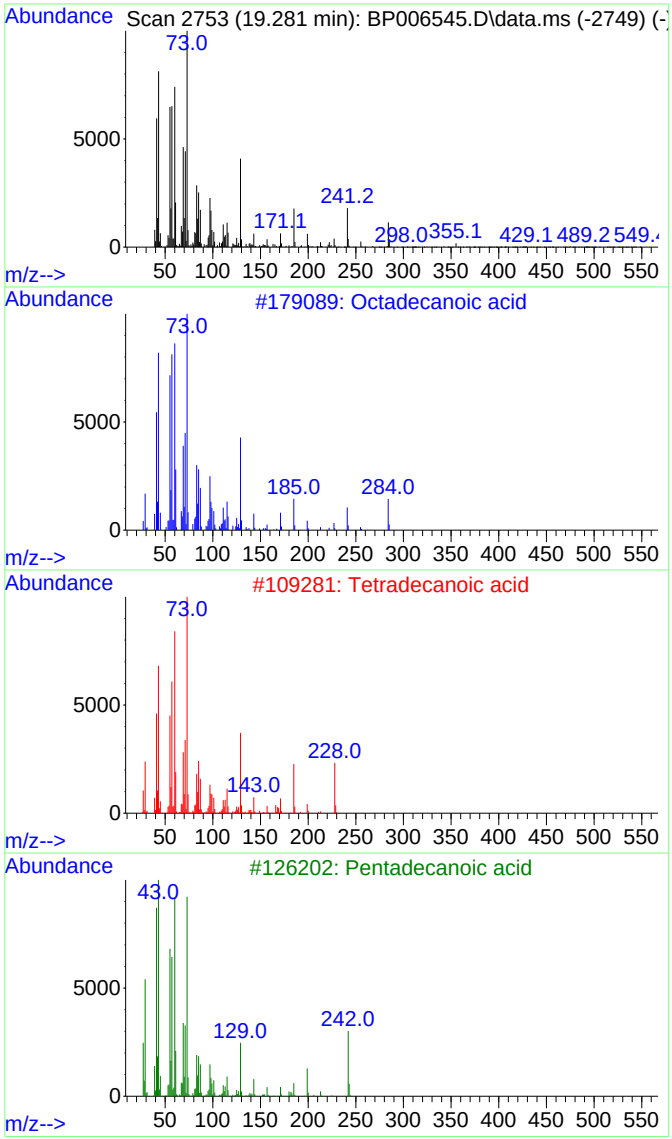
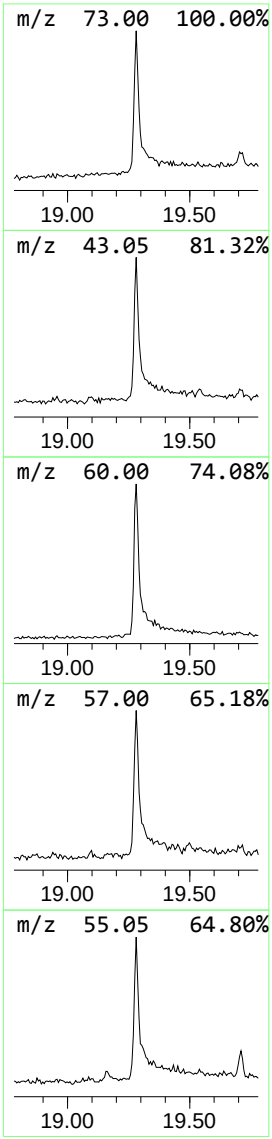
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.281	5.71 ng	599262	Chrysene-d12	21.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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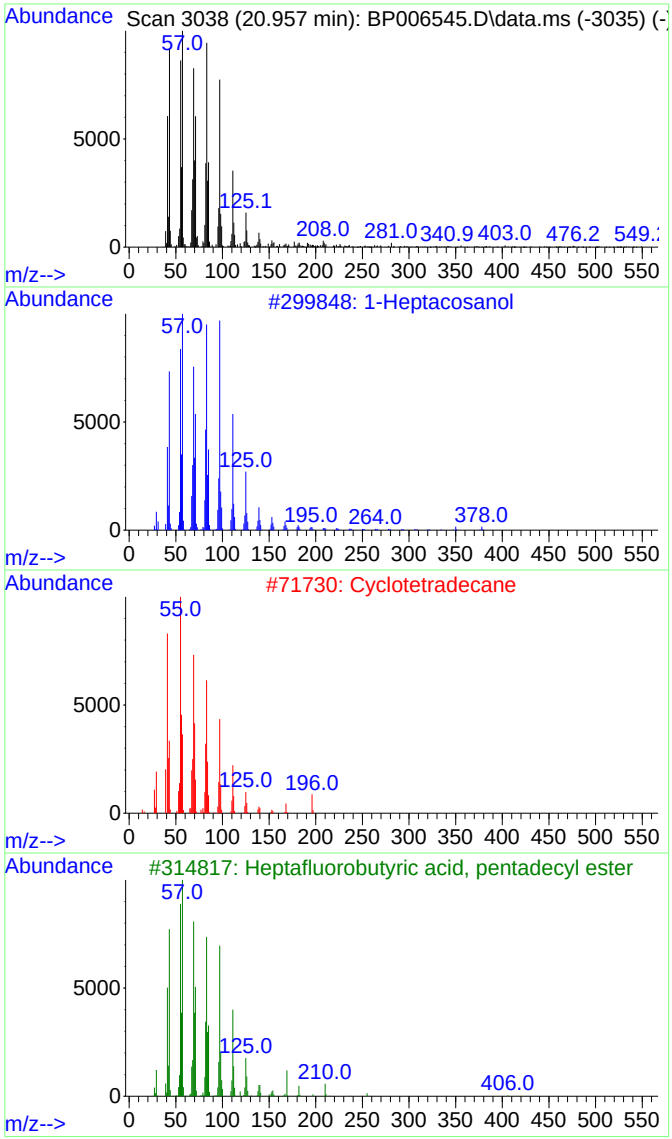
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

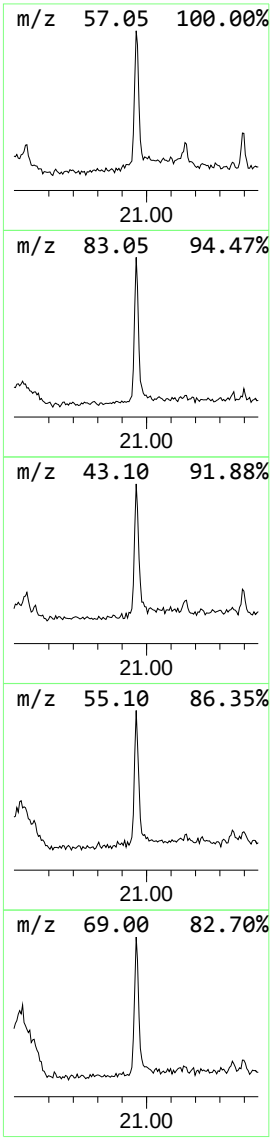
****

Peak Number 6 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	3.40 ng	356309	Chrysene-d12	21.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	Cyclotetradecane	196	C14H28	000295-17-0	93
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-...	4.905	35.0	ng	2004230	1	7.752	1144640	20.0
2-Pentanone, 4-...	5.970	7.7	ng	438941	1	7.752	1144640	20.0
Ethanol, 2-(2-b...	10.328	7.0	ng	546899	2	10.534	1552690	20.0
n-Hexadecanoic ...	18.040	6.1	ng	578611	4	17.134	1901760	20.0
Octadecanoic acid	19.281	5.7	ng	599262	5	21.233	2097510	20.0
1-Heptacosanol	20.957	3.4	ng	356309	5	21.233	2097510	20.0