LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007165.D
Acq On : 24 Sep 2021 18:49
Operator : CG/JU
Sample : M3775-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PE-4

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-BP092121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007165.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.999	319	325	337	rBV	275447	406564	4.53%	0.760%
2	5.463	397	404	413	rBV	2874145	4126967	46.00%	7.715%
3	7.057	667	675	691	rBV	2725881	4309420	48.04%	8.056%
4	7.887	808	816	824	rBV	953647	1445463	16.11%	2.702%
5	9.051	1004	1014	1029	rBV	1614016	2786564	31.06%	5.209%
6	10.475	1250	1256	1266	rBV	115066	220998	2.46%	0.413%
7	10.687	1282	1292	1304	rBV	1202874	2069531	23.07%	3.869%
8	13.145	1702	1710	1725	rBV	4494128	6553614	73.05%	12.251%
9	14.369	1911	1918	1937	rVV	193934	542875	6.05%	1.015%
10	14.516	1937	1943	1963	rVB	1798588	2854566	31.82%	5.336%
11	16.010	2190	2197	2211	rBV	3567632	5310200	59.19%	9.927%
12	17.269	2405	2411	2416	rBV	2275123	3273417	36.49%	6.119%
13	17.310	2416	2418	2425	rVB	124212	144362	1.61%	0.270%
14	18.157	2556	2562	2573	rBV2	647278	1017517	11.34%	1.902%
15	19.274	2748	2752	2759	rVB	343557	443777	4.95%	0.830%
16	19.386	2767	2771	2781	rBV2	228050	384645	4.29%	0.719%
17	19.627	2808	2812	2820	rVB	282045	382062	4.26%	0.714%
18	19.827	2840	2846	2851	rBV	7547962	8971351	100.00%	16.771%
19	21.063	3052	3056	3064	rBV2	544396	708646	7.90%	1.325%
20	21.351	3100	3105	3109	rBV	2893704	3796155	42.31%	7.096%
21	23.762	3509	3515	3528	rVB2	1807679	3744711	41.74%	7.000%

Sum of corrected areas: 53493405

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Misc :
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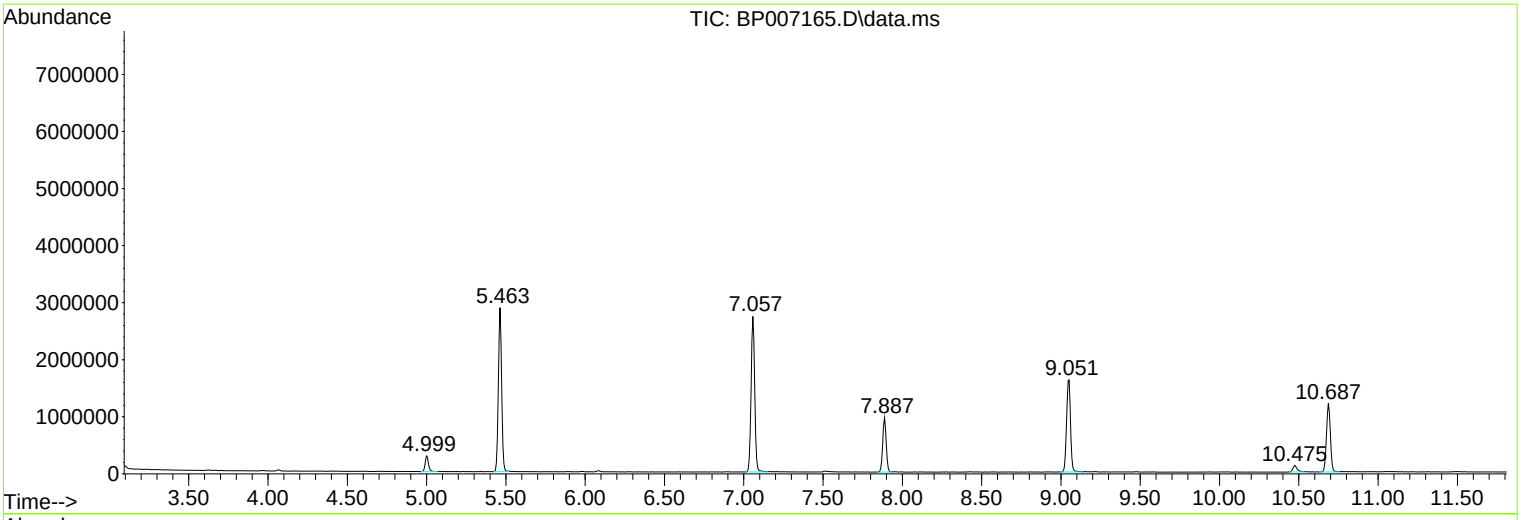
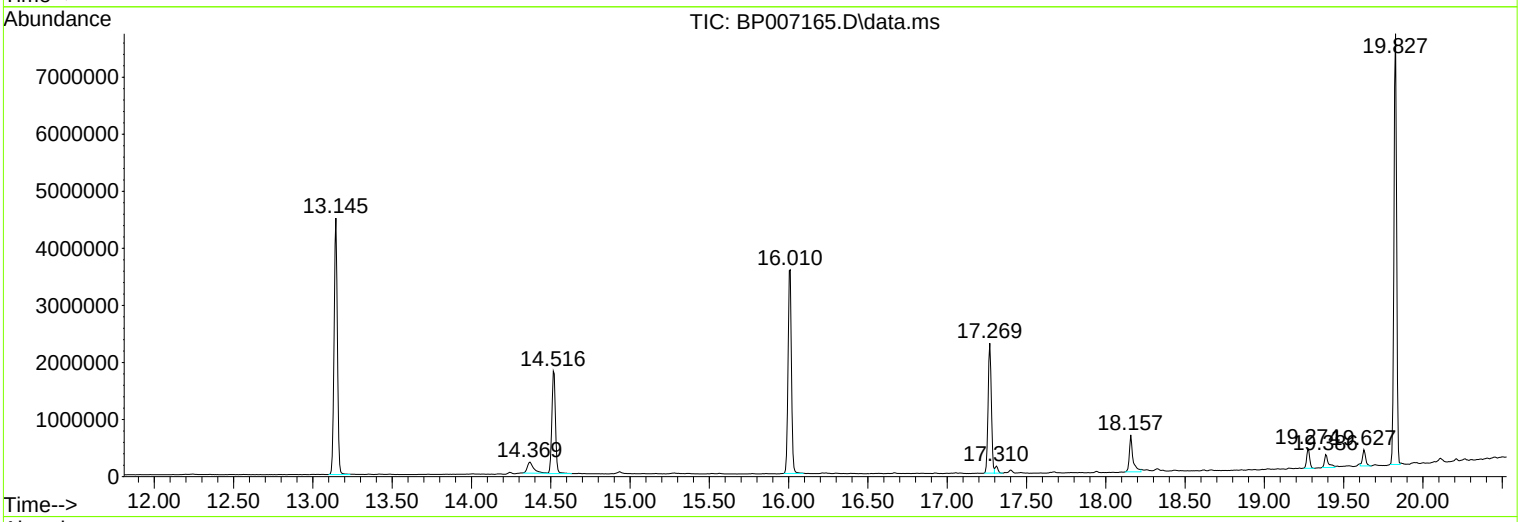
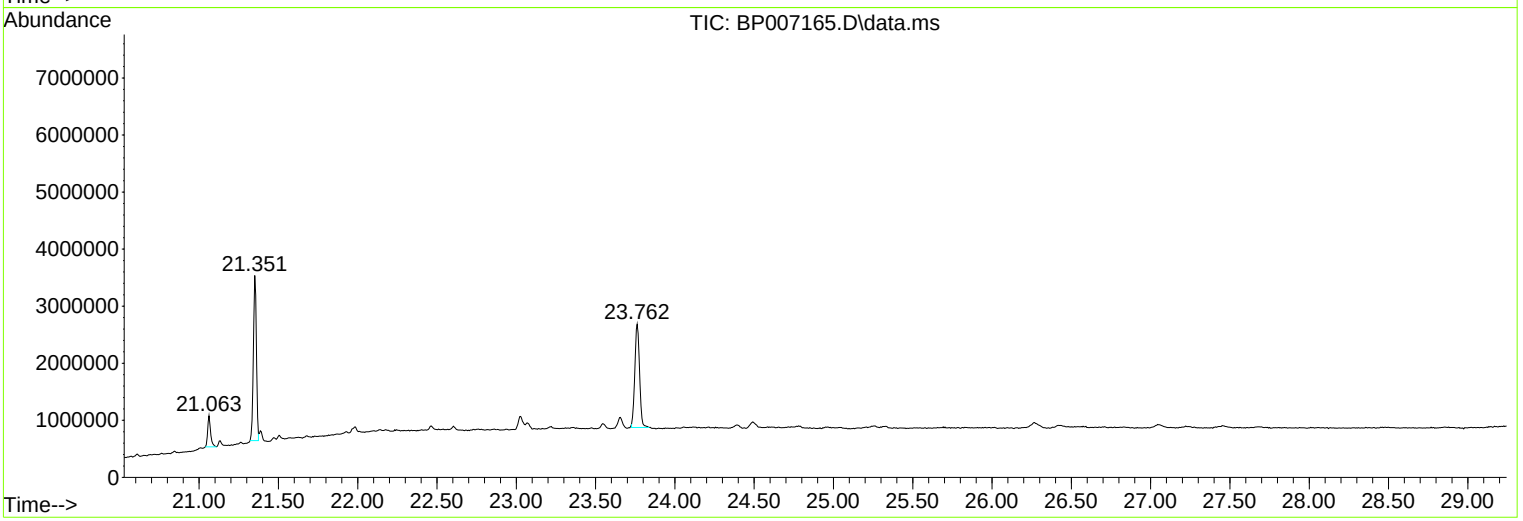
Instrument : BNA_P
ClientSampleId : PE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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TIC Library : C:\Database\NIST20.L
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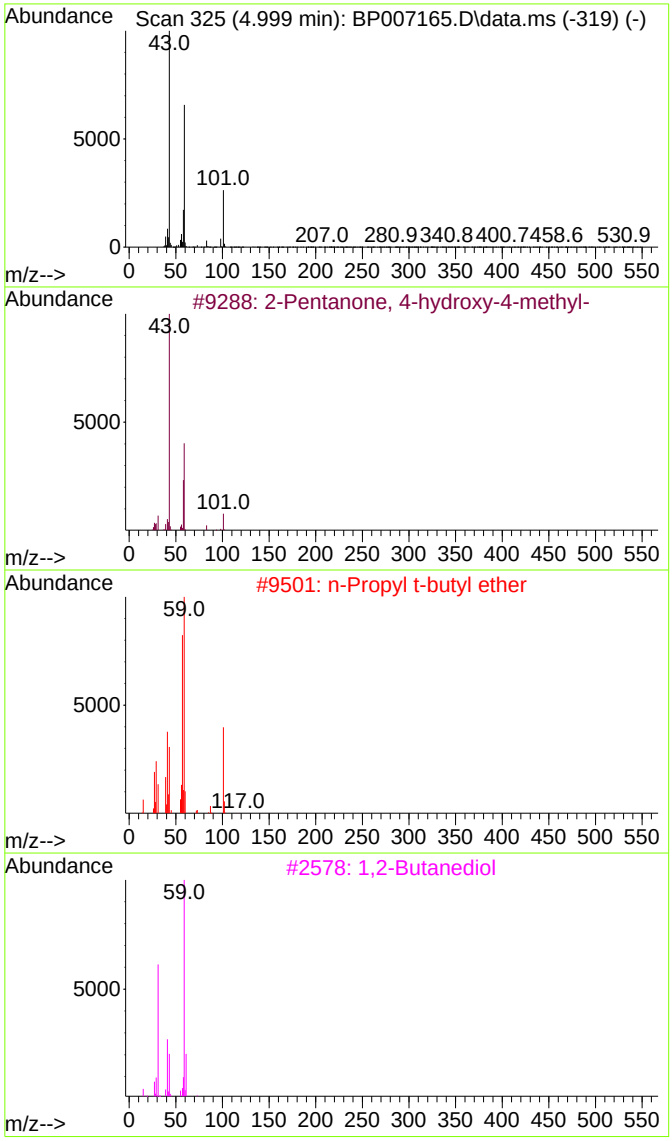
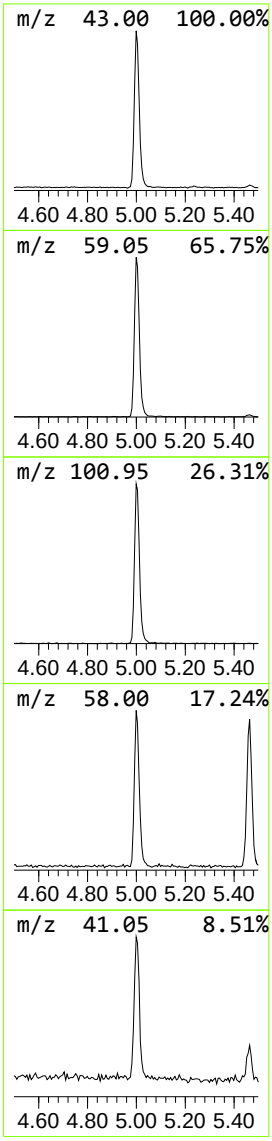
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.999	5.63 ng	406564	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	1,2-Butanediol	90	C4H10O2	000584-03-2	17
4	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	17
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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Misc :
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Instrument : BNA_P
ClientSampleId : PE-4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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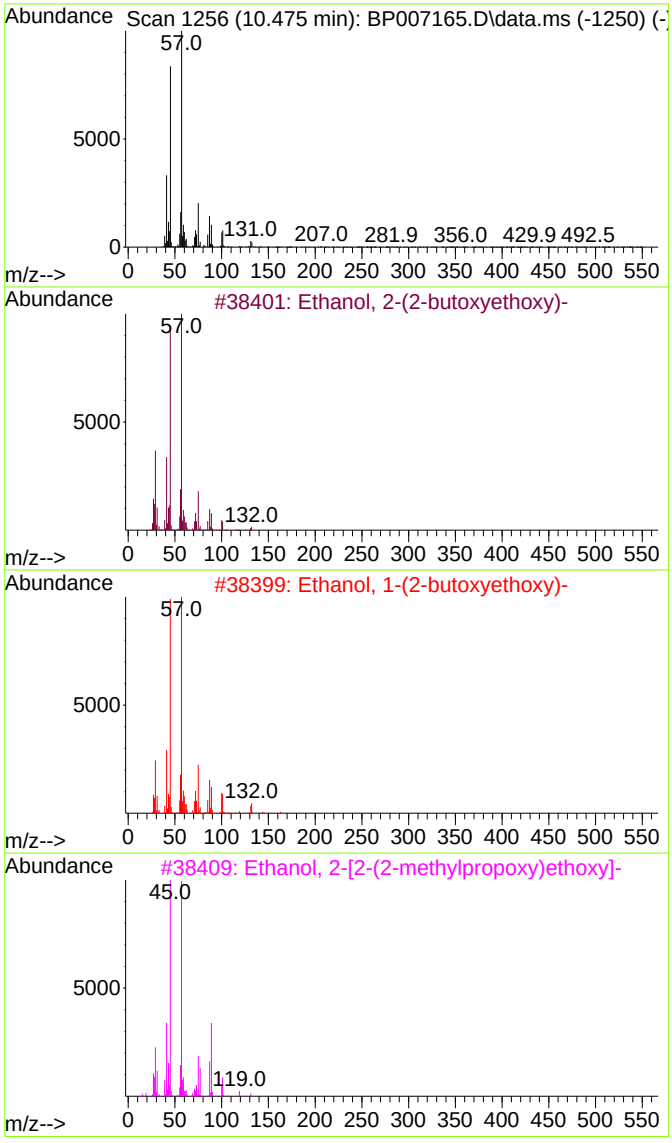
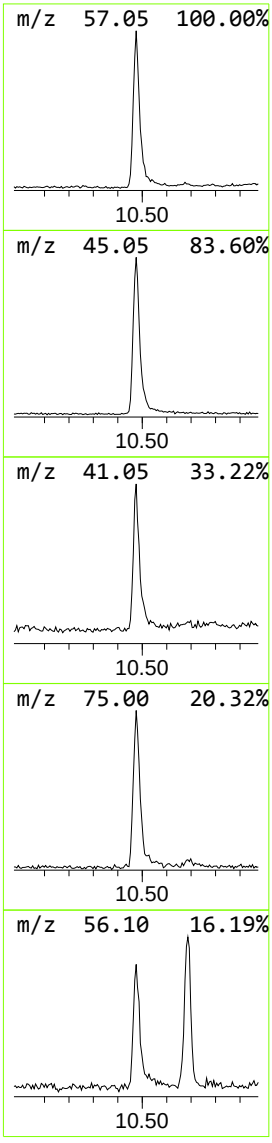
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	2.14 ng	220998	Naphthalene-d8	10.687

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	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59





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Acq On : 24 Sep 2021 18:49
Operator : CG/JU
Sample : M3775-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
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TIC Library : C:\Database\NIST20.L
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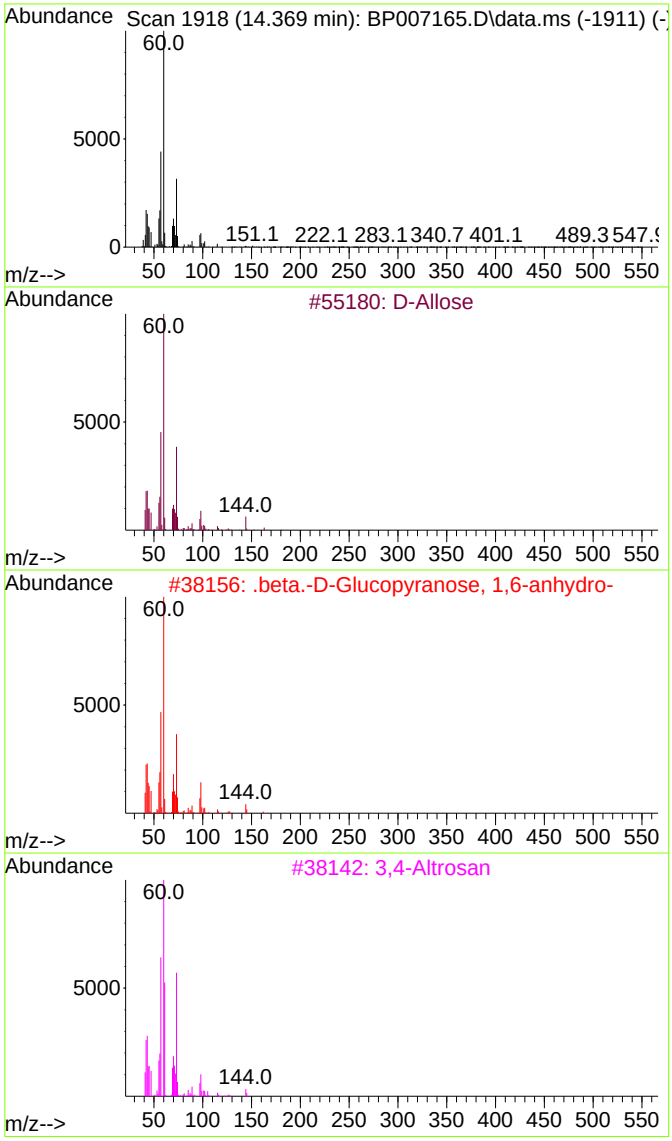
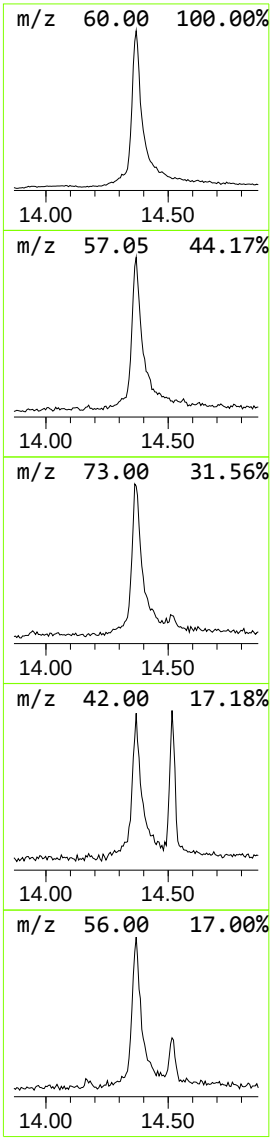
Peak Number 3 D-Allose Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.369	3.80 ng	542875	Acenaphthene-d10	14.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Allose	180	C6H12O6	002595-97-3	90
2	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	78
3	3,4-Altrosan	162	C6H10O5	1000129-76-4	58
4	Butanoic acid	88	C4H8O2	000107-92-6	53
5	.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	53





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Sample : M3775-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
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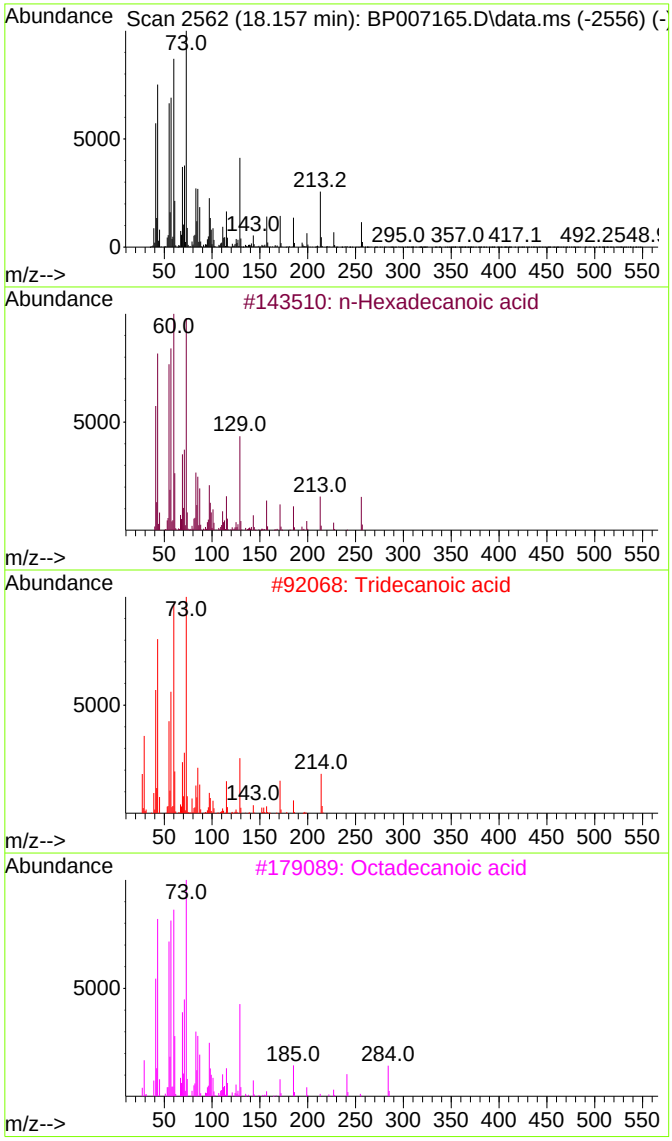
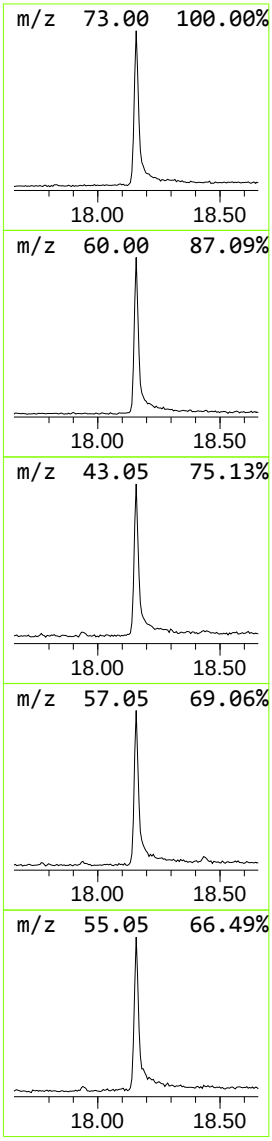
Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	6.22 ng	1017520	Phenanthrene-d10	17.269

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	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	90





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Data File : BP007165.D
Acq On : 24 Sep 2021 18:49
Operator : CG/JU
Sample : M3775-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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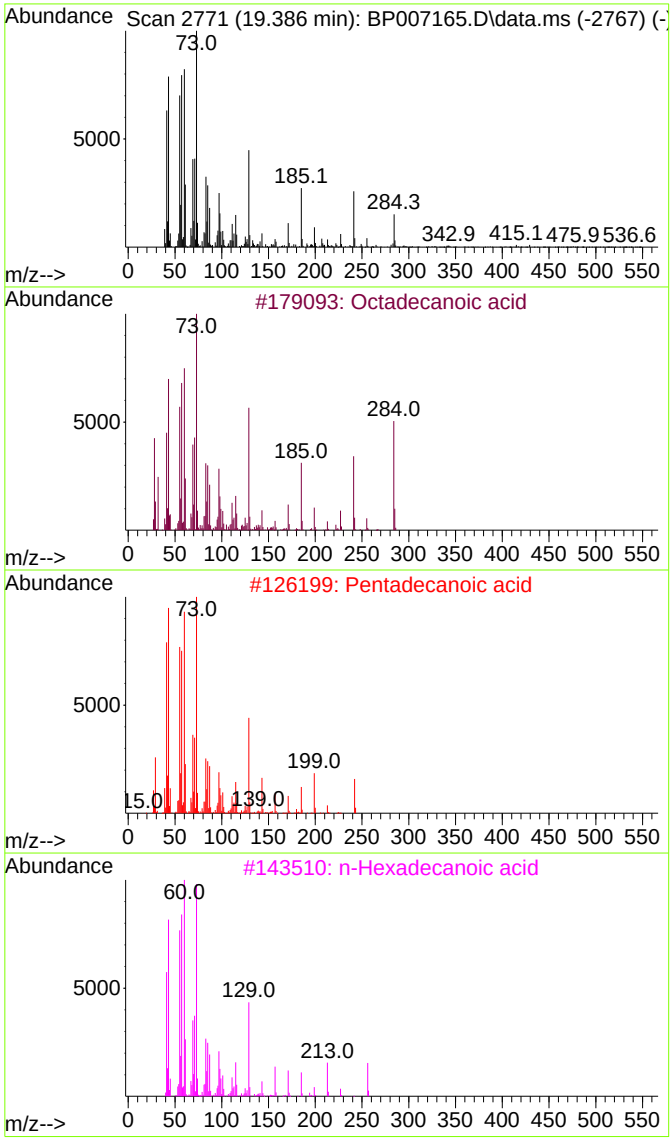
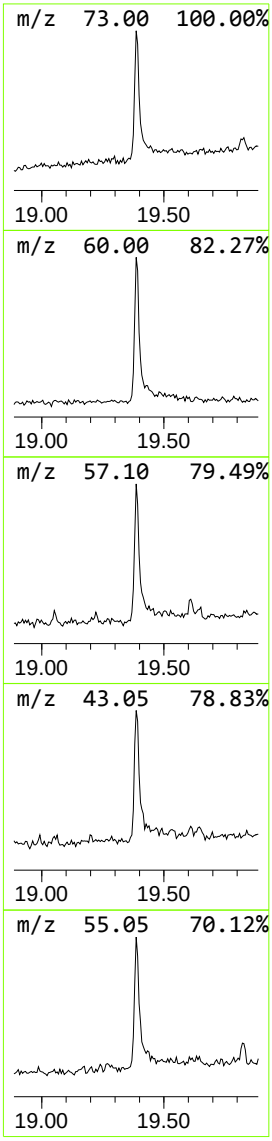
Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	2.03 ng	384645	Chrysene-d12	21.351

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	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Sample : M3775-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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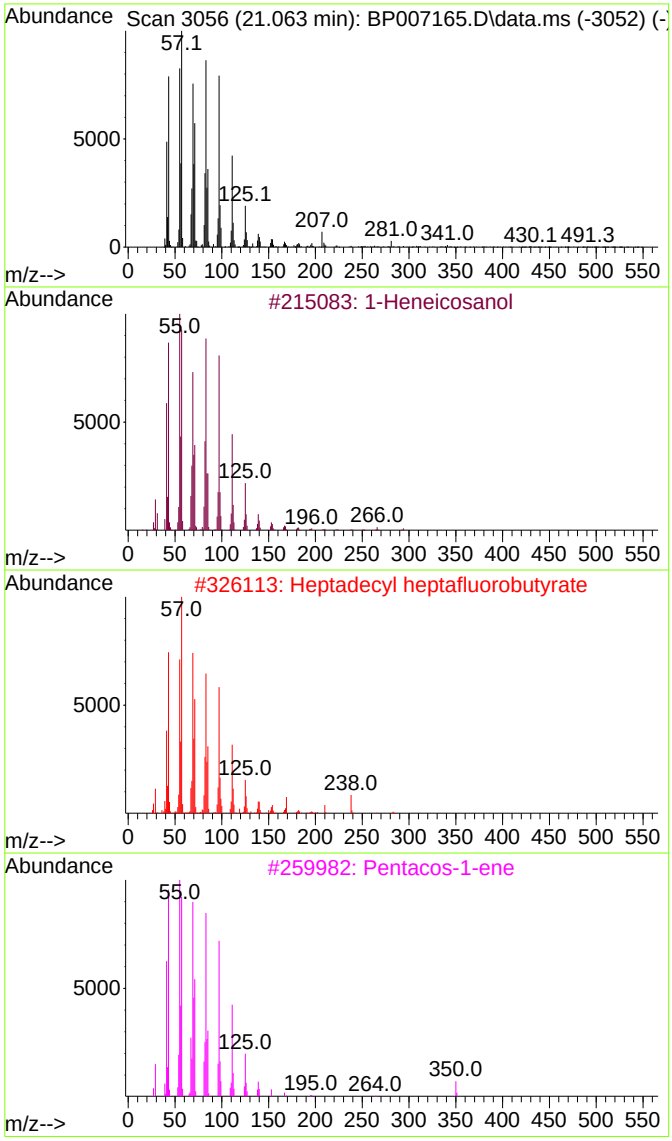
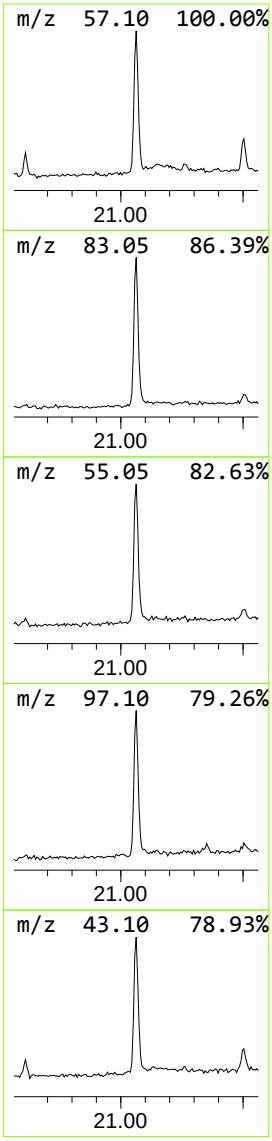
Peak Number 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	3.73 ng	708646	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Pentacos-1-ene	350	C25H50	016980-85-1	94
4	Cyclopentadecane	210	C15H30	000295-48-7	93
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	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-...	4.999	5.6	ng	406564	1	7.887	1445460	20.0
Ethanol, 2-(2-b...	10.475	2.1	ng	220998	2	10.687	2069530	20.0
D-Allose	14.369	3.8	ng	542875	3	14.516	2854570	20.0
n-Hexadecanoic ...	18.157	6.2	ng	1017520	4	17.269	3273420	20.0
Octadecanoic acid	19.386	2.0	ng	384645	5	21.351	3796160	20.0
1-Heneicosanol	21.063	3.7	ng	708646	5	21.351	3796160	20.0