LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007167.D
Acq On : 24 Sep 2021 19:57
Operator : CG/JU
Sample : M3775-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PE-2D

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: BP007167.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.005	321	326	334	rVB	337756	500813	4.41%	0.813%
2	5.463	397	404	417	rBV	3577979	5259273	46.28%	8.533%
3	7.057	667	675	690	rBV	3364731	5428939	47.77%	8.809%
4	7.887	808	816	823	rBV	967298	1492571	13.13%	2.422%
5	9.046	1005	1013	1025	rBV	2035418	3490611	30.71%	5.664%
6	10.475	1248	1256	1265	rBV	147152	293224	2.58%	0.476%
7	10.687	1284	1292	1304	rBV	1275106	2151711	18.93%	3.491%
8	13.145	1703	1710	1725	rBV	5686541	8461826	74.46%	13.729%
9	14.363	1911	1917	1933	rBV2	124150	351652	3.09%	0.571%
10	14.516	1937	1943	1963	rVB	1888410	2885610	25.39%	4.682%
11	16.004	2190	2196	2216	rVB	4303128	6386510	56.20%	10.362%
12	17.269	2404	2411	2416	rBV	2290308	3262670	28.71%	5.294%
13	17.310	2416	2418	2423	rVB	121004	136348	1.20%	0.221%
14	18.157	2556	2562	2576	rBV	708724	1122030	9.87%	1.821%
15	19.274	2748	2752	2759	rVB	300024	385825	3.39%	0.626%
16	19.386	2767	2771	2783	rBV3	352012	561014	4.94%	0.910%
17	19.627	2808	2812	2821	rVB	237759	345967	3.04%	0.561%
18	19.827	2840	2846	2851	rBV	9183964	11364583	100.00%	18.439%
19	21.063	3052	3056	3064	rVB3	456767	571515	5.03%	0.927%
20	21.351	3100	3105	3109	rBV	2854682	3633121	31.97%	5.895%
21	23.762	3509	3515	3523	rVB2	1794491	3546661	31.21%	5.755%

Sum of corrected areas: 61632474

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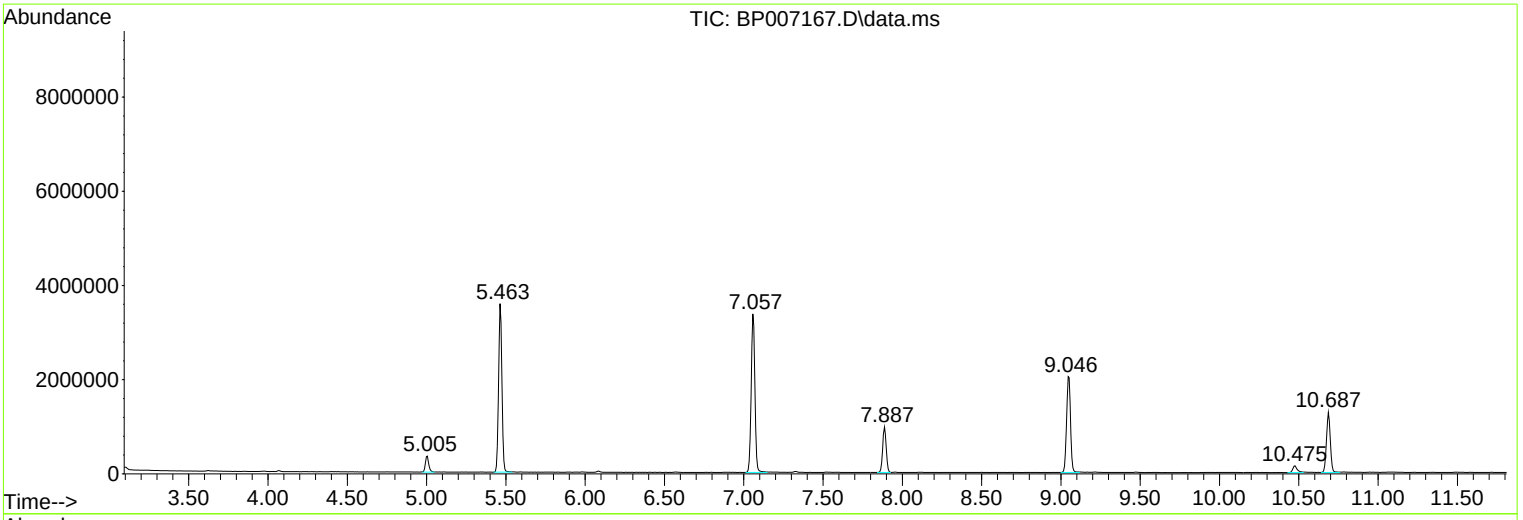
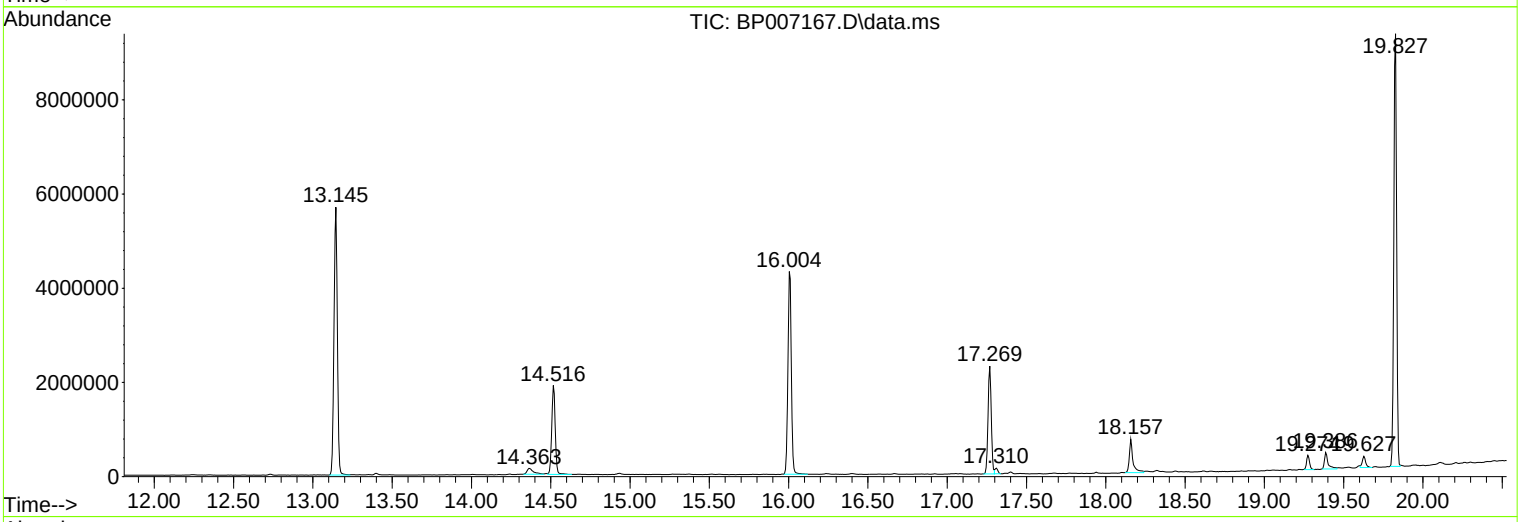
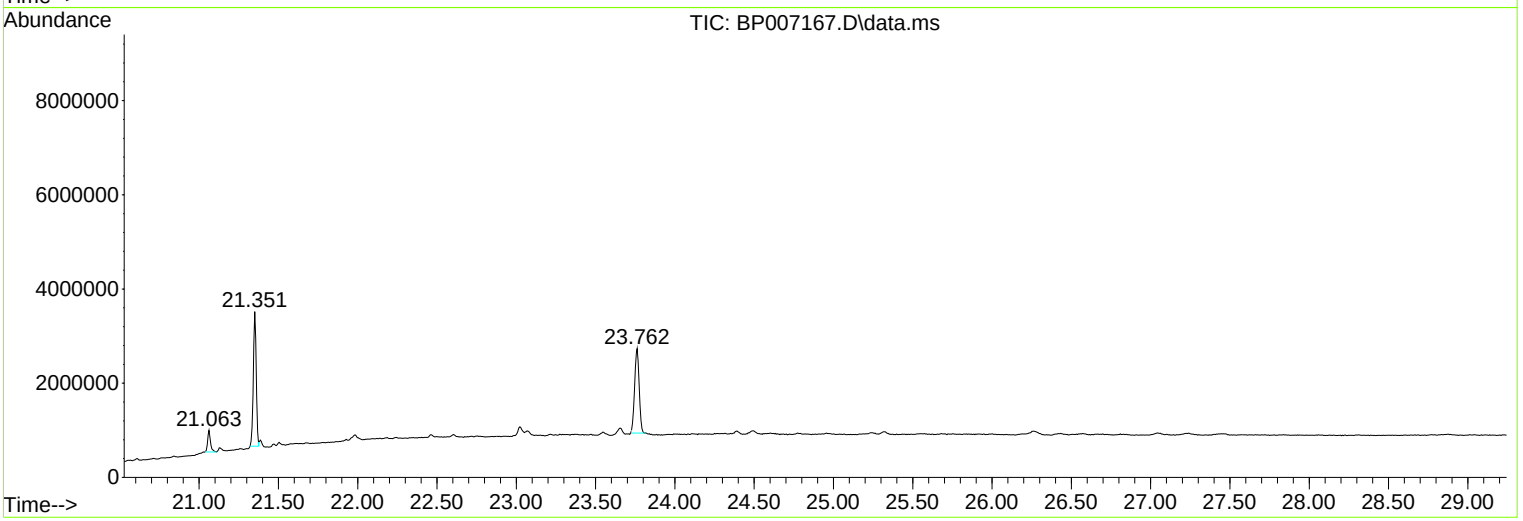
Instrument :
BNA_P
ClientSampleId :
PE-2D

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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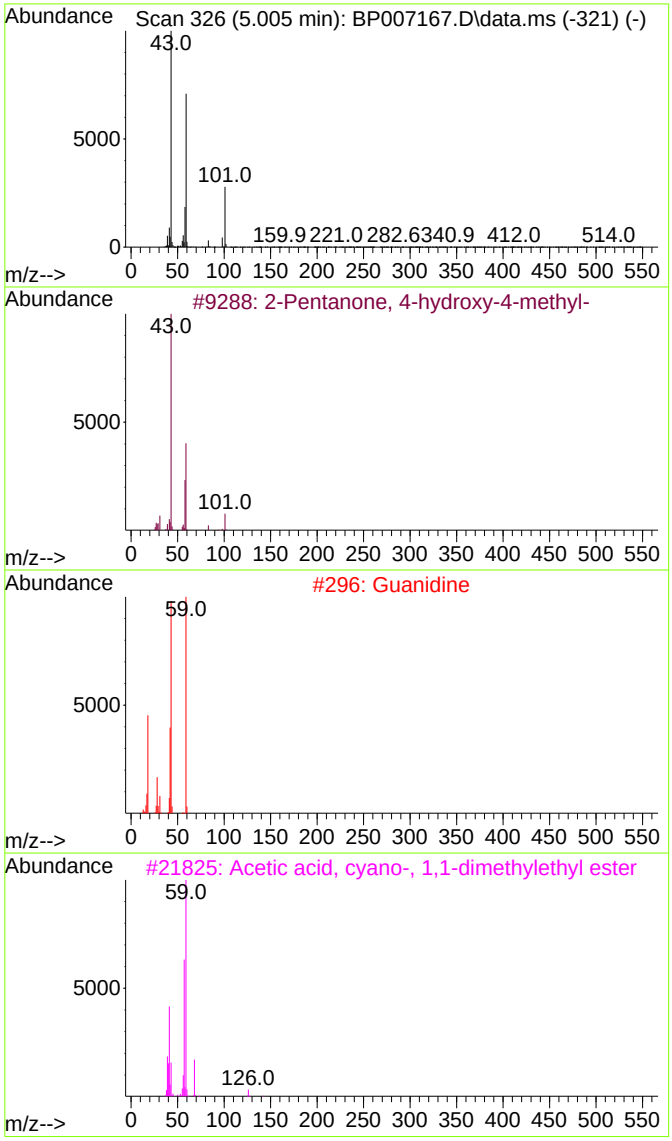
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

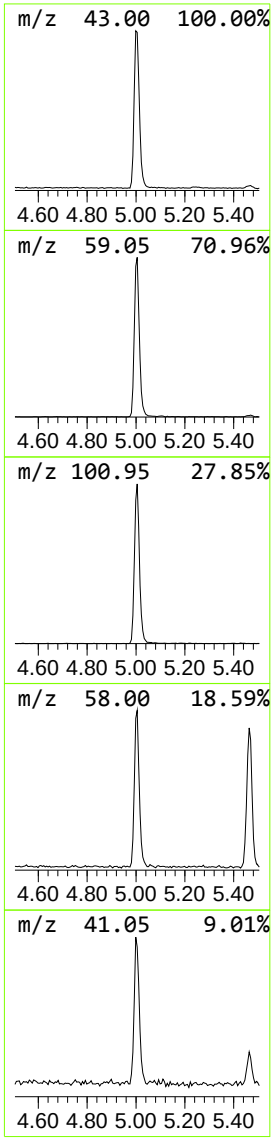
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.005	6.71 ng	500813	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	Guanidine	59	CH5N3	000113-00-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Instrument :
BNA_P
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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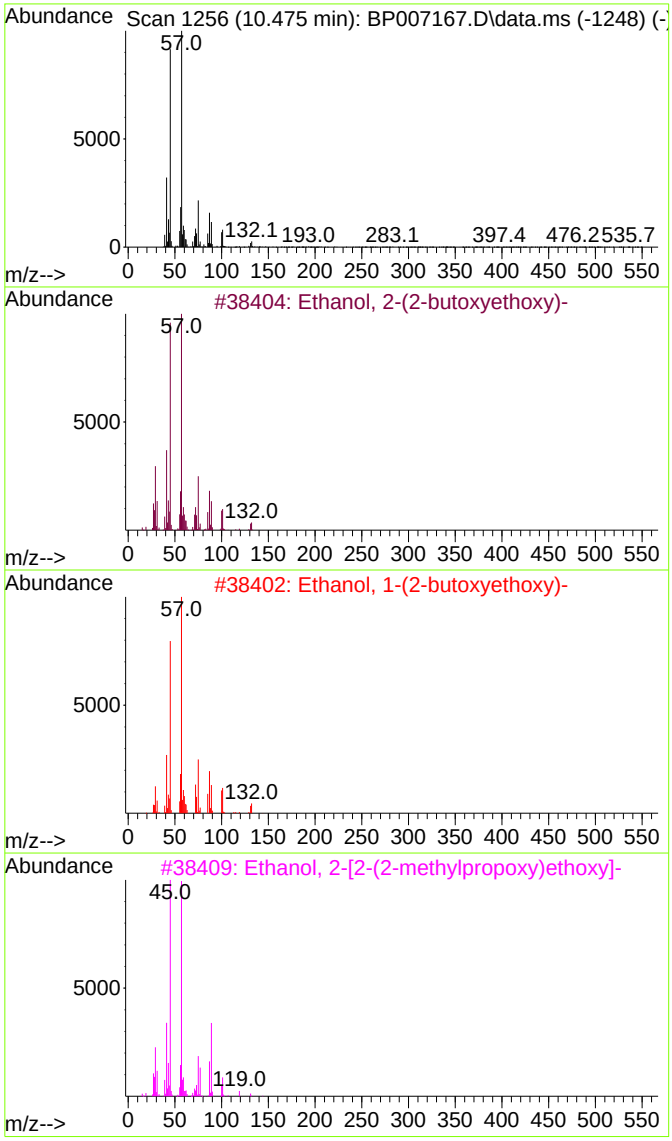
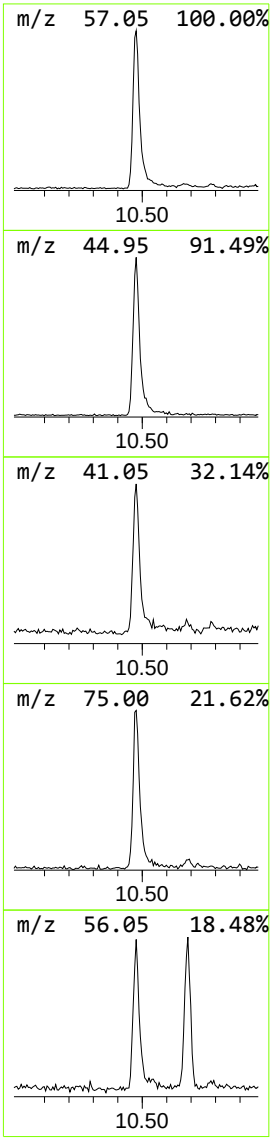
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	2.73 ng	293224	Naphthalene-d8	10.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	2-Propanol, 1-(2-butoxyethoxy)-	176	C9H20O3	000124-16-3	50





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Acq On : 24 Sep 2021 19:57
Operator : CG/JU
Sample : M3775-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PE-2D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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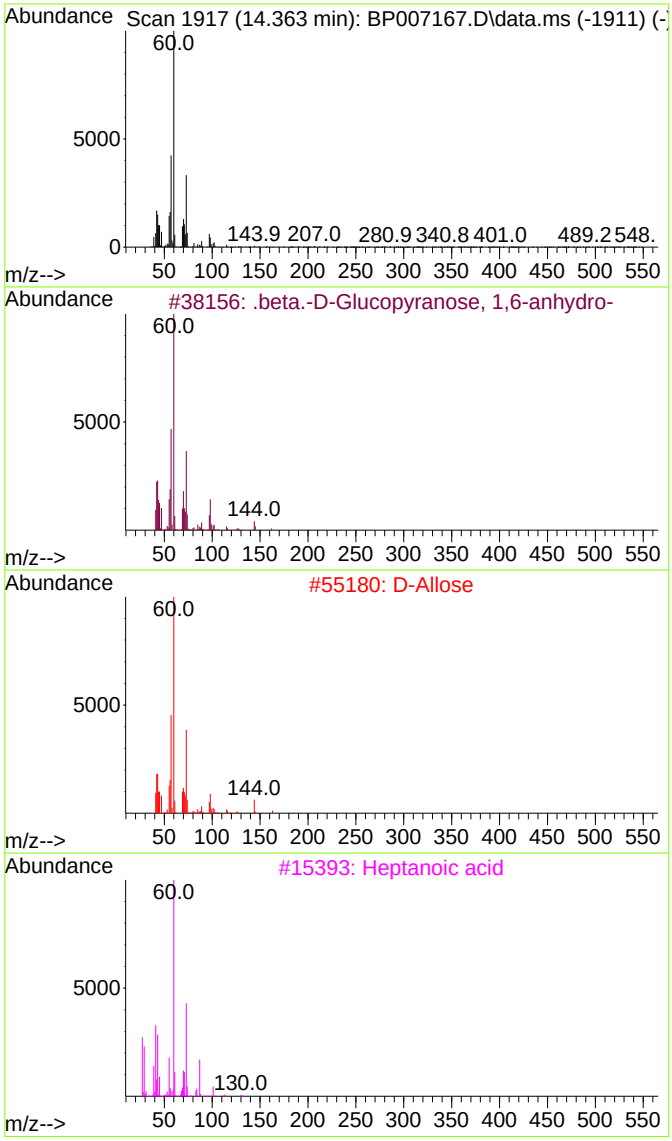
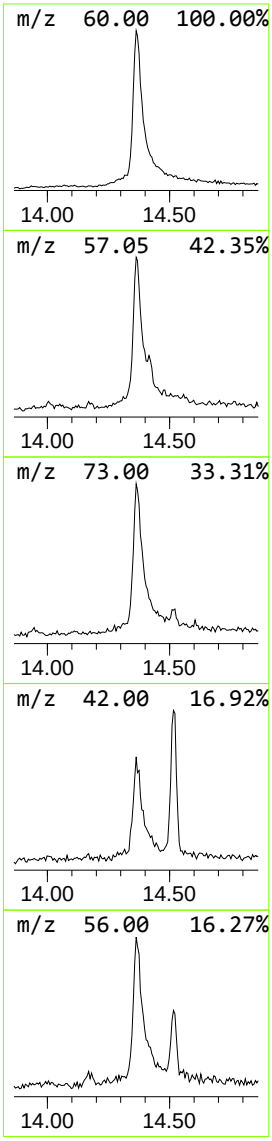
****
Peak Number 3 .beta.-D-Glucopyranose, 1,6... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.363	2.44 ng	351652	Acenaphthene-d10	14.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	90
2	D-Allose	180	C6H12O6	002595-97-3	90
3	Heptanoic acid	130	C7H14O2	000111-14-8	64
4	Butanoic acid	88	C4H8O2	000107-92-6	53
5	Pentanoic acid	102	C5H10O2	000109-52-4	50





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Sample : M3775-03
Misc :
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Instrument :
BNA_P
ClientSampleId :
PE-2D

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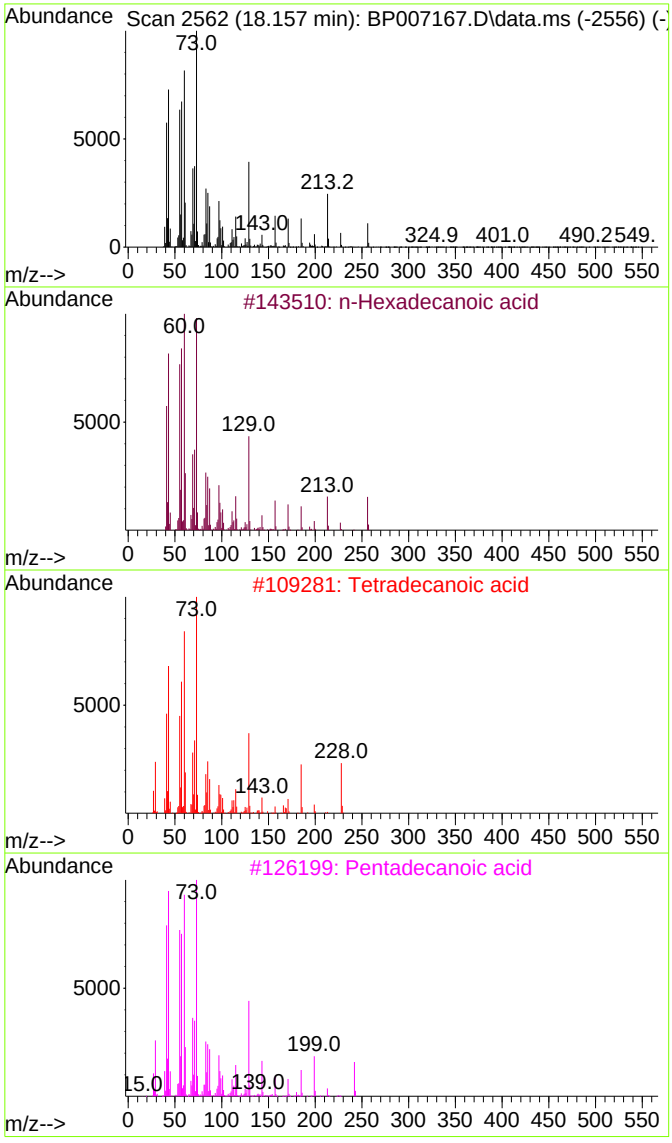
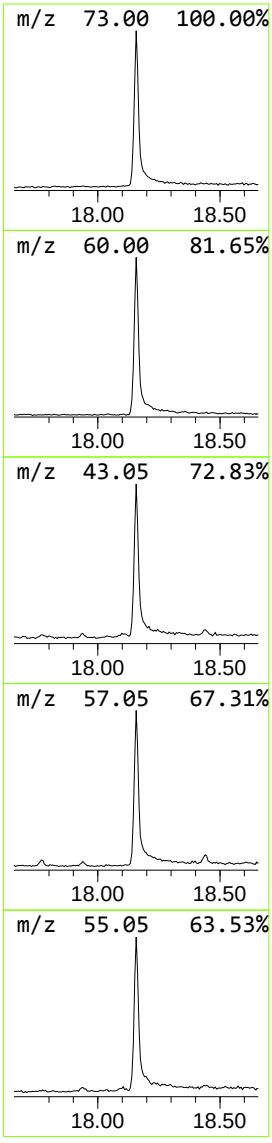
Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	6.88 ng	1122030	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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Sample : M3775-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PE-2D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
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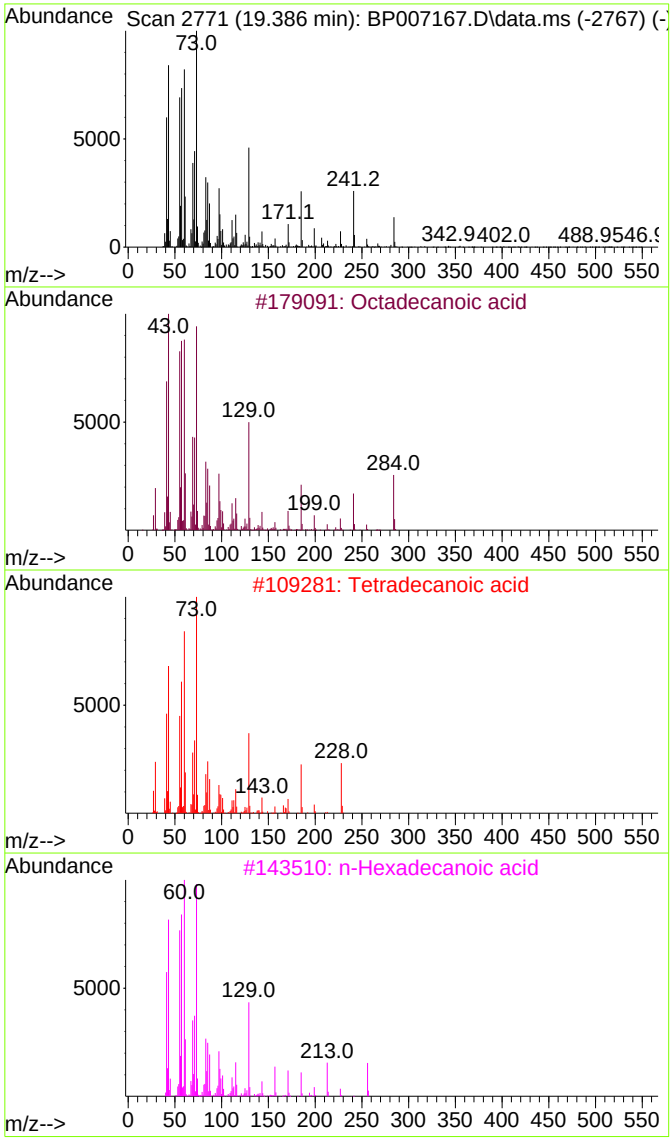
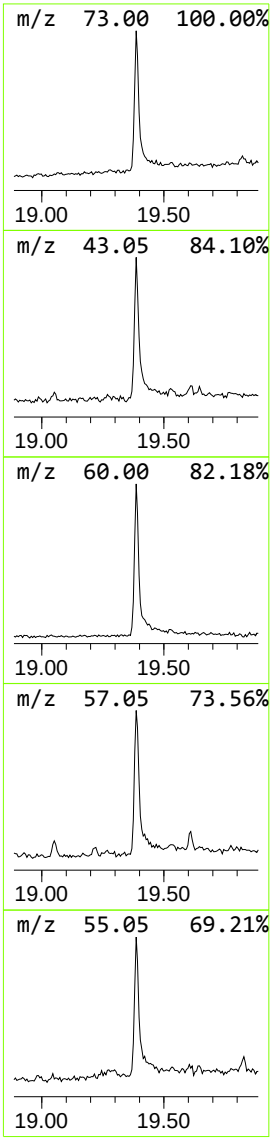
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	3.09 ng	561014	Chrysene-d12	21.351

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	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	68





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Instrument : BNA_P
ClientSampleId : PE-2D

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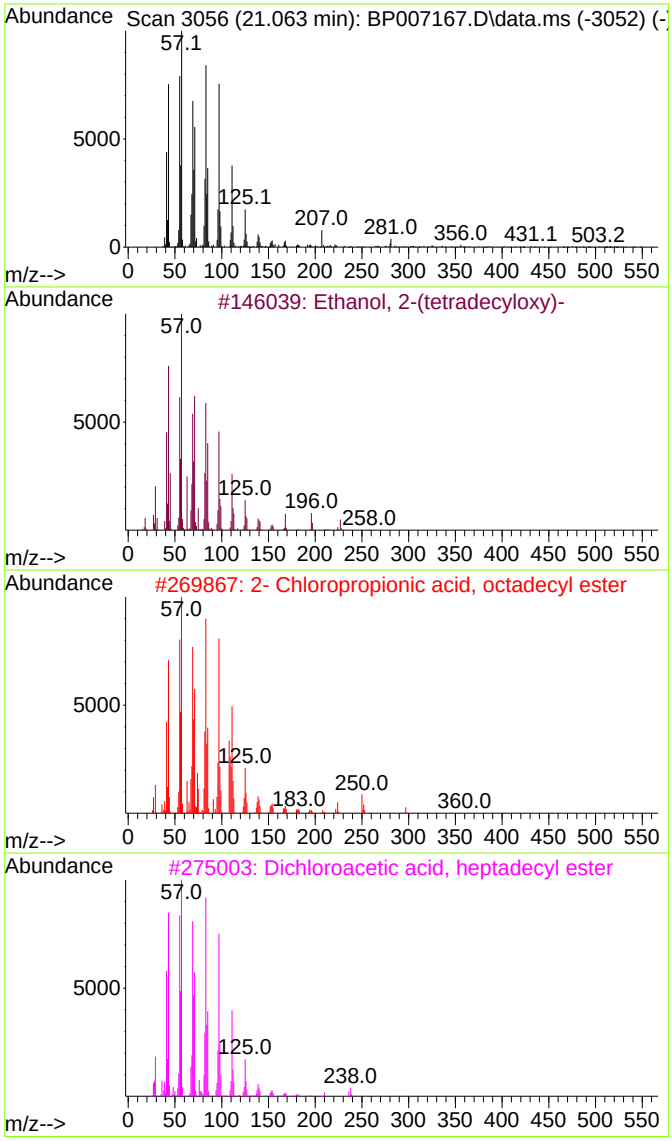
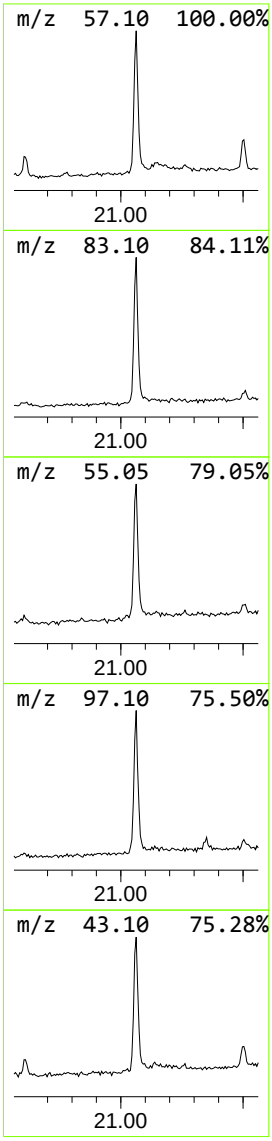
****

Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	3.15 ng	571515	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	97
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	96
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Cyclotetracosane	336	C24H48	000297-03-0	93





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-...	5.005	6.7	ng	500813	1	7.887	1492570	20.0
Ethanol, 2-(2-b...	10.475	2.7	ng	293224	2	10.687	2151710	20.0
.beta.-D-Glucop...	14.363	2.4	ng	351652	3	14.516	2885610	20.0
n-Hexadecanoic ...	18.157	6.9	ng	1122030	4	17.269	3262670	20.0
Octadecanoic acid	19.386	3.1	ng	561014	5	21.351	3633120	20.0
Ethanol, 2-(tet...	21.063	3.1	ng	571515	5	21.351	3633120	20.0