LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007164.D
Acq On : 24 Sep 2021 18:15
Operator : CG/JU
Sample : M3775-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PE-3

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: BP007164.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	333	rBV	313097	443491	4.77%	0.714%
2	5.464	397	404	415	rBV	2983031	4321257	46.50%	6.960%
3	7.058	667	675	693	rBV	2903387	4628002	49.80%	7.454%
4	7.887	805	816	823	rBV	911597	1402582	15.09%	2.259%
5	9.046	1004	1013	1022	rBV	1720353	2897992	31.18%	4.668%
6	10.469	1248	1255	1266	rBV	152360	292798	3.15%	0.472%
7	10.687	1283	1292	1302	rBV	1176193	1993902	21.45%	3.212%
8	11.034	1345	1351	1366	rBV	104523	322893	3.47%	0.520%
9	13.146	1703	1710	1719	rBV	4631225	6786470	73.02%	10.931%
10	14.387	1902	1921	1926	rBV	344098	1048338	11.28%	1.689%
11	14.440	1926	1930	1938	rVV	662834	1185092	12.75%	1.909%
12	14.516	1938	1943	1962	rVB	1809782	2828710	30.44%	4.556%
13	14.934	2009	2014	2026	rVB	97509	160488	1.73%	0.258%
14	16.010	2190	2197	2210	rVB	4035324	5808087	62.50%	9.355%
15	16.928	2347	2353	2368	rBV	511682	971470	10.45%	1.565%
16	17.269	2405	2411	2416	rBV	2265731	3175696	34.17%	5.115%
17	18.163	2557	2563	2585	rBV	2332798	3431454	36.92%	5.527%
18	18.886	2682	2686	2701	rBV	341205	653799	7.03%	1.053%
19	19.275	2749	2752	2760	rVB	122230	171449	1.84%	0.276%
20	19.392	2767	2772	2783	rBV	1253182	1728417	18.60%	2.784%
21	19.828	2841	2846	2851	rBV	7770091	9293648	100.00%	14.969%
22	20.416	2943	2946	2949	rBV	136988	178196	1.92%	0.287%
23	21.063	3052	3056	3063	rBV2	539264	690288	7.43%	1.112%
24	21.351	3100	3105	3110	rBV	2795854	3643949	39.21%	5.869%
25	23.763	3509	3515	3536	rVB2	1912906	4027316	43.33%	6.487%

Sum of corrected areas: 62085784

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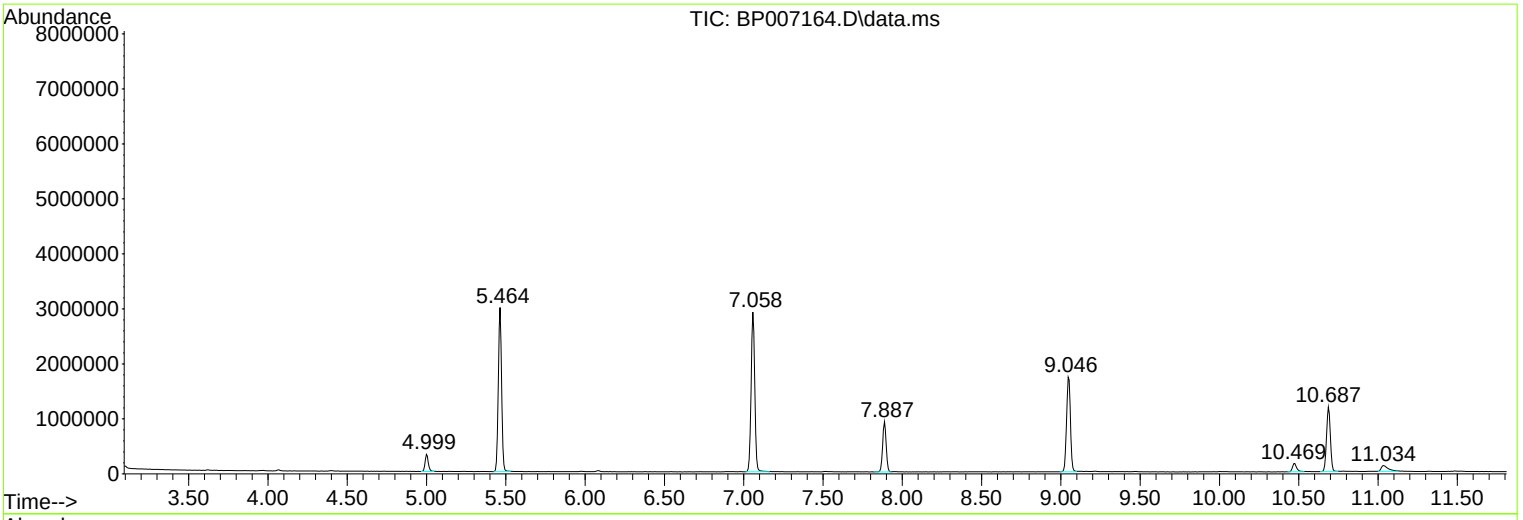
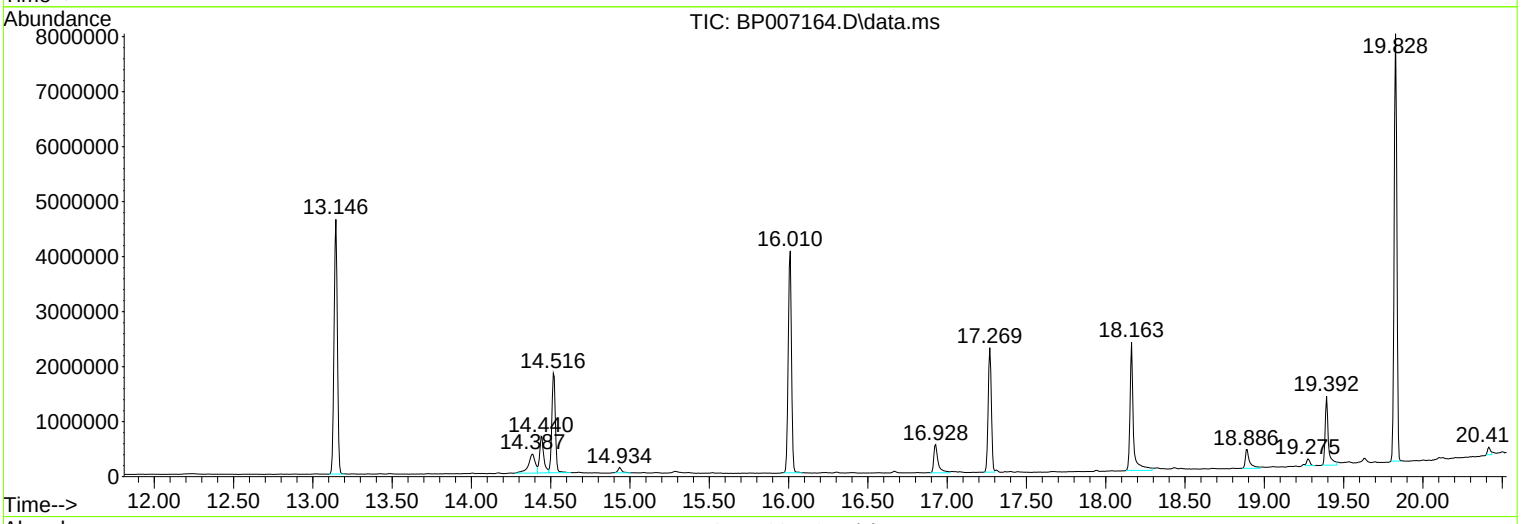
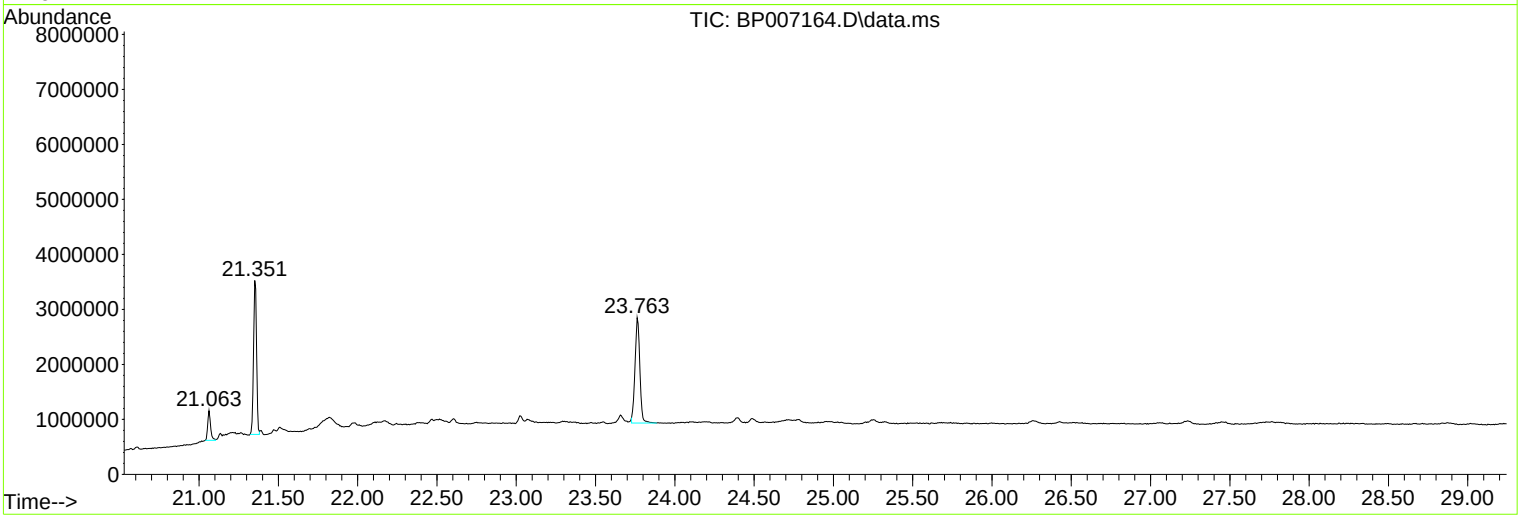
Instrument :
BNA_P
ClientSampleId :
PE-3

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

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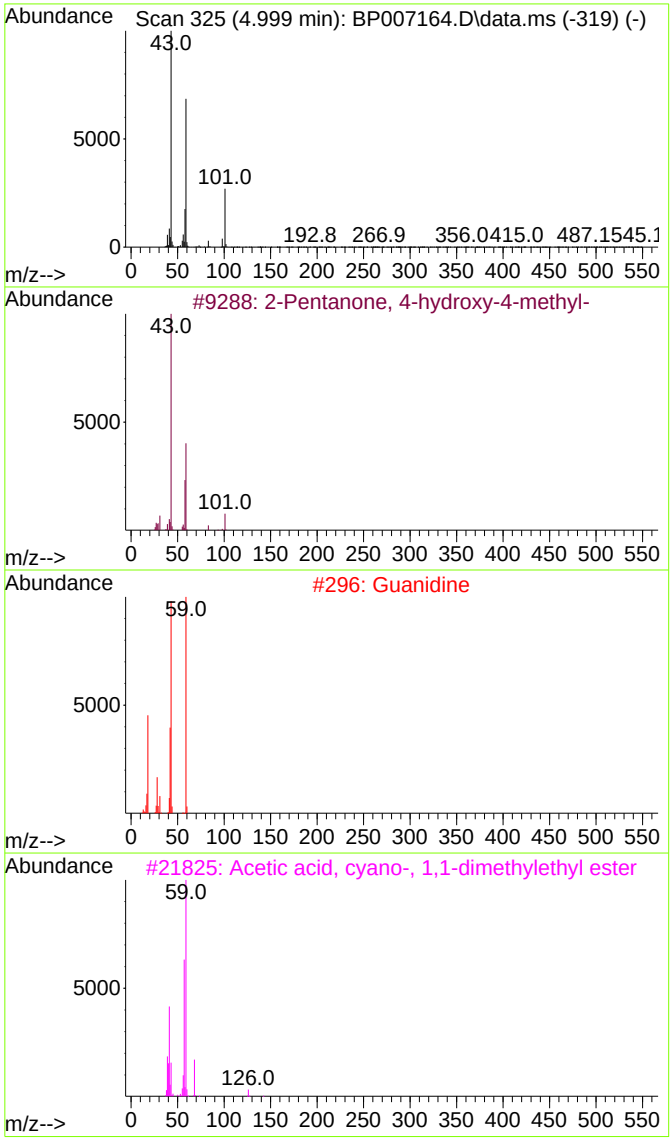
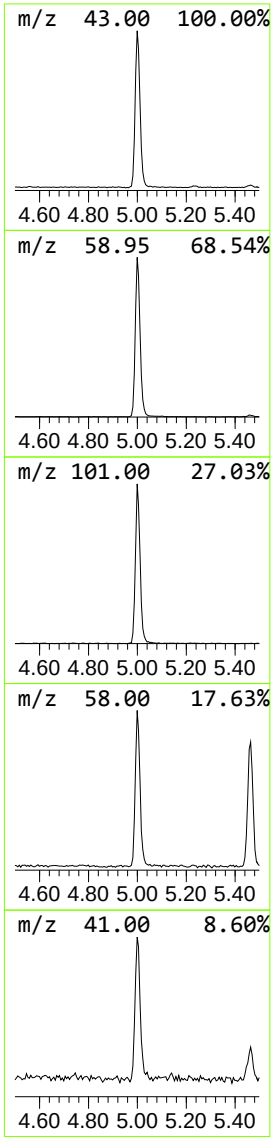
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.999	6.32 ng	443491	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	1,2-Butanediol	90	C4H10O2	000584-03-2	17
5	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	17





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Data File : BP007164.D
Acq On : 24 Sep 2021 18:15
Operator : CG/JU
Sample : M3775-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PE-3

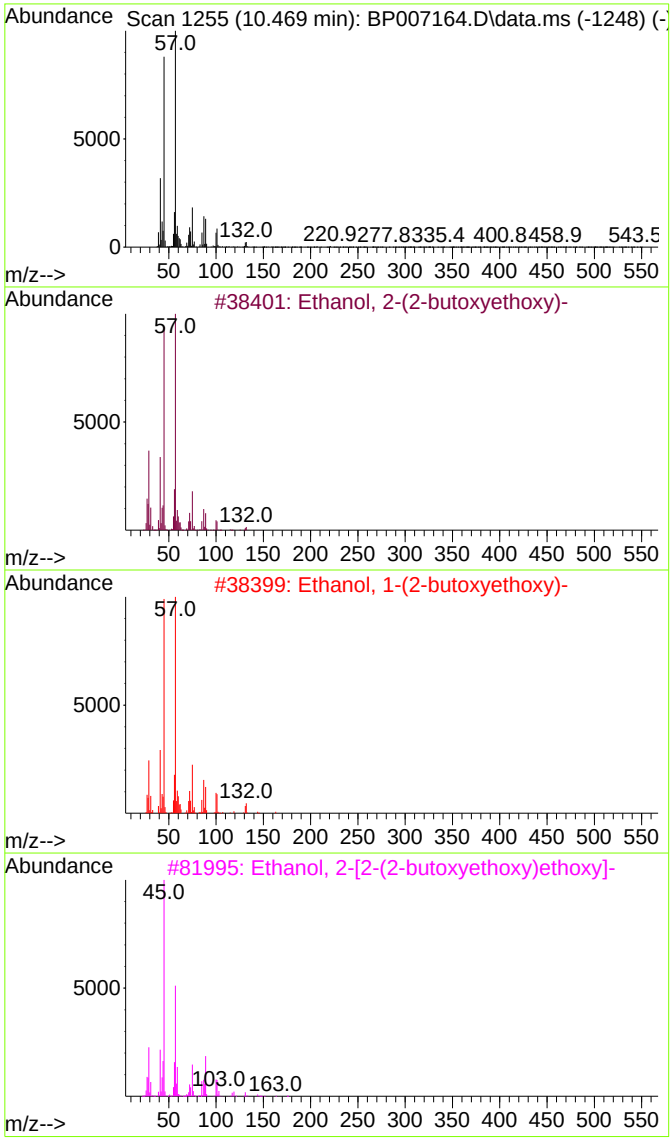
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

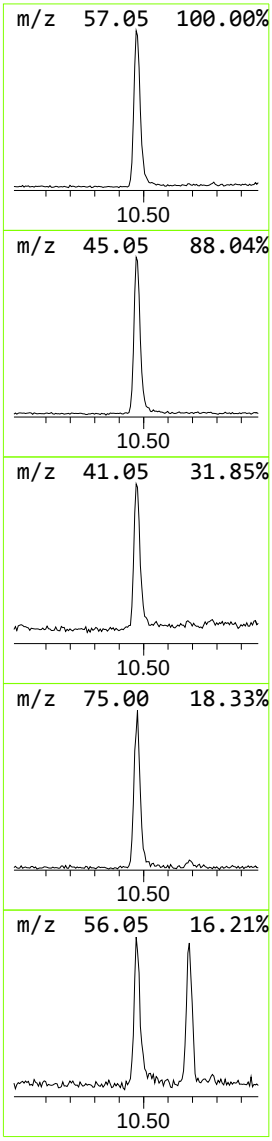
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	2.94 ng	292798	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-butoxyethoxy)et...	206	C10H22O4	000143-22-6	72
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	68
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52





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Sample : M3775-04
Misc :
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Instrument : BNA_P
ClientSampleId : PE-3

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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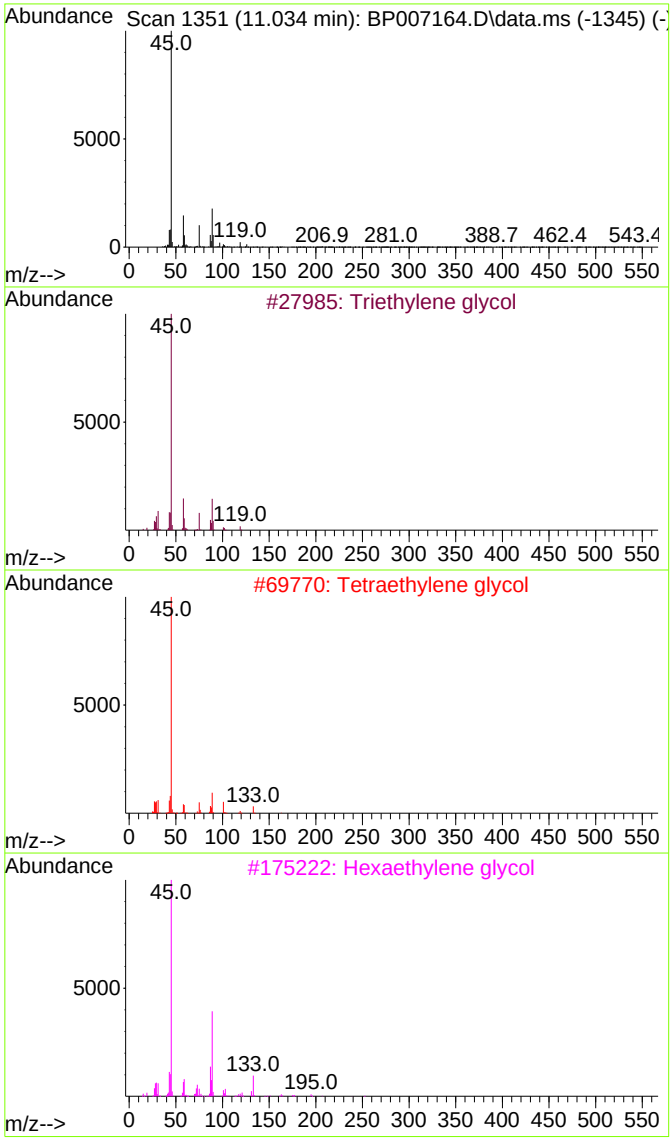
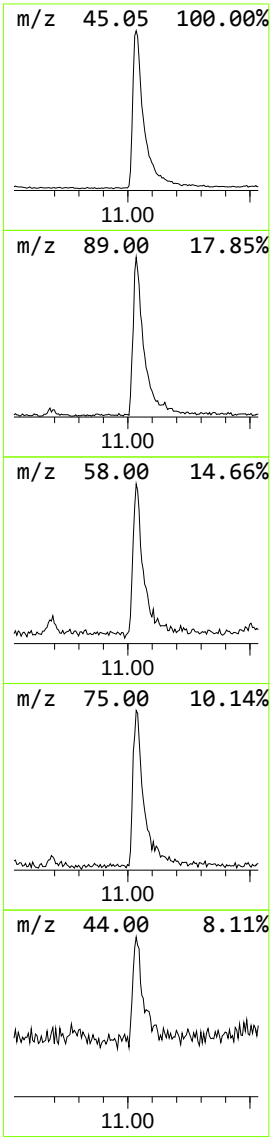
Peak Number 3 Triethylene glycol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.034	3.24 ng	322893	Naphthalene-d8	10.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethylene glycol	150	C6H14O4	000112-27-6	90
2	Tetraethylene glycol	194	C8H18O5	000112-60-7	64
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	50
4	Acetaldehyde, tetramer	176	C8H16O4	000108-62-3	42
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	40





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Operator : CG/JU
Sample : M3775-04
Misc :
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Instrument : BNA_P
ClientSampleId : PE-3

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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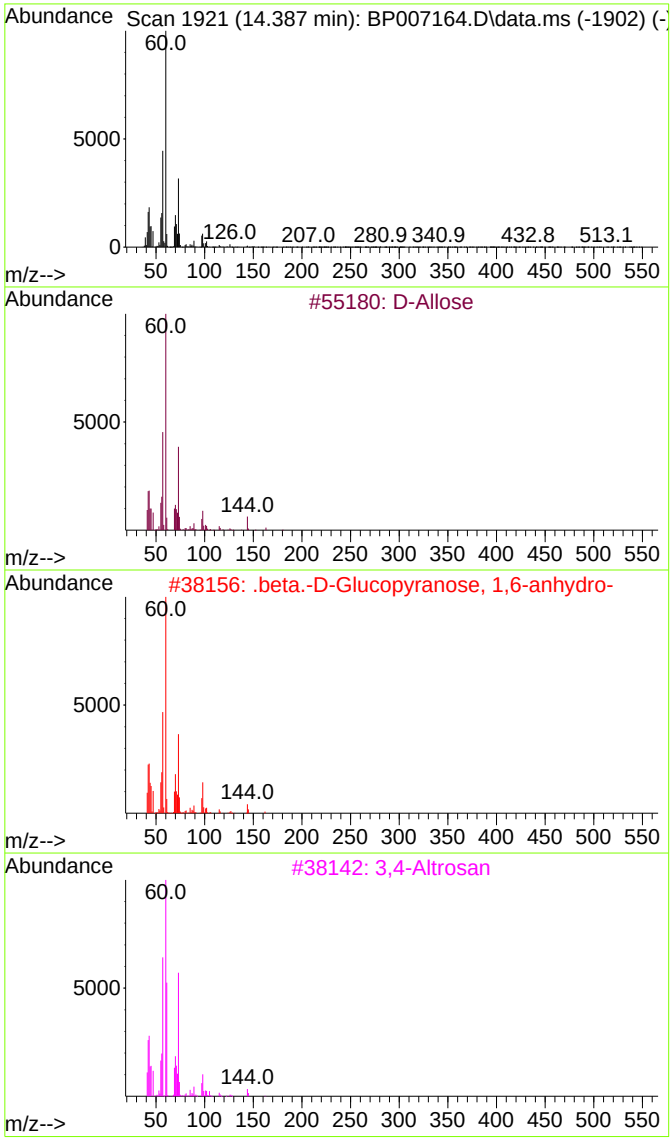
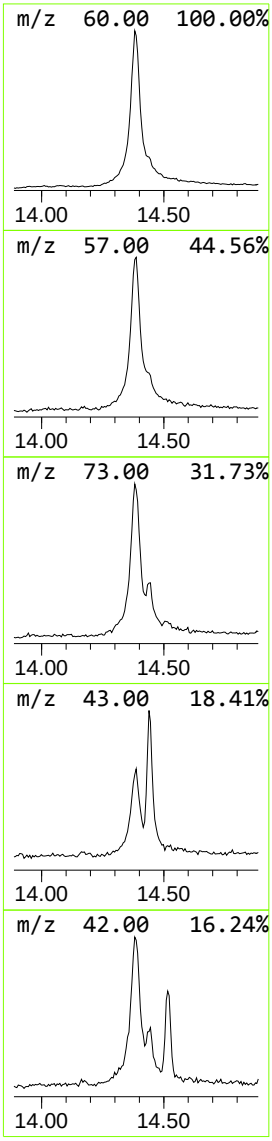
Peak Number 4 D-Allose Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.387	7.41 ng	1048340	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	90
3	3,4-Altrosan	162	C6H10O5	1000129-76-4	86
4	Rhamnose	164	C6H12O5	003615-41-6	50
5	Heptanoic acid	130	C7H14O2	000111-14-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
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Acq On : 24 Sep 2021 18:15
Operator : CG/JU
Sample : M3775-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PE-3

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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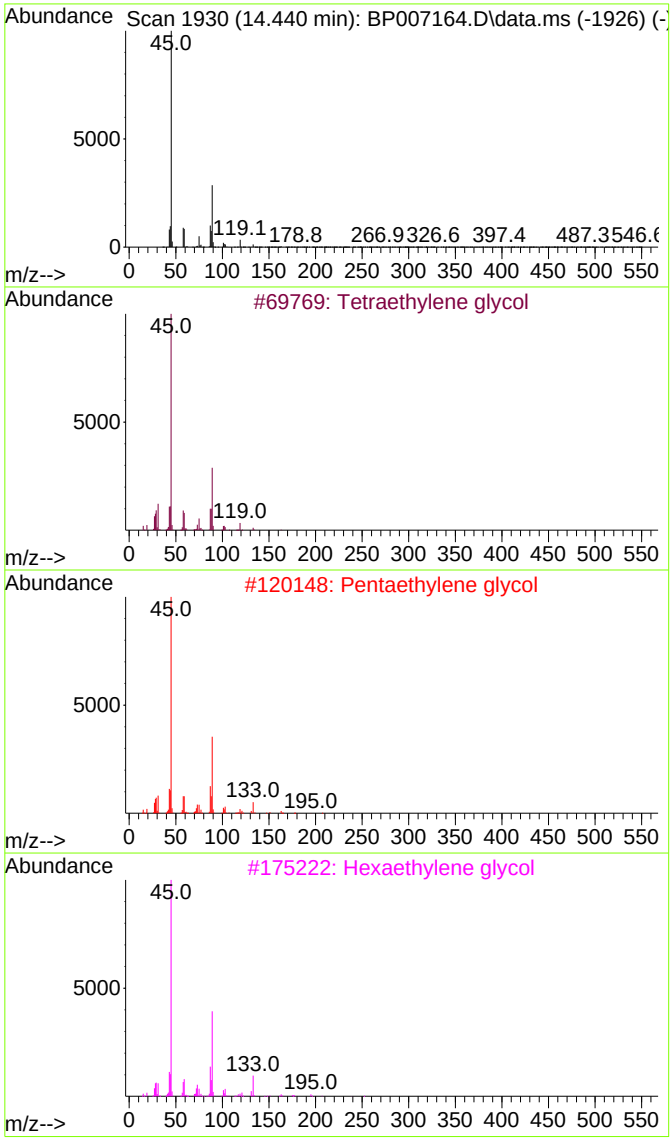
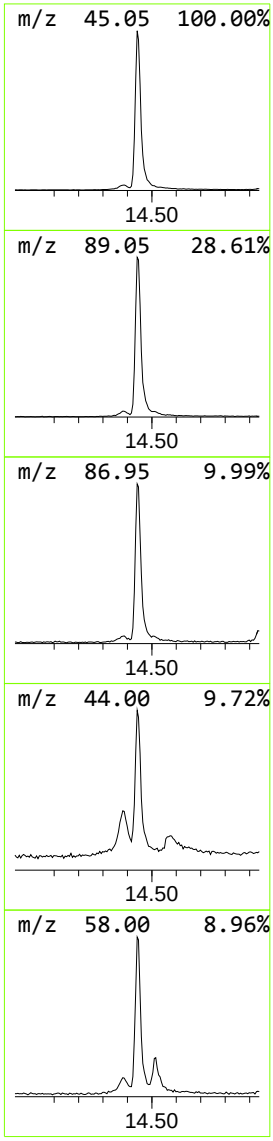
****

Peak Number 5 Tetraethylene glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.440	8.38 ng	1185090	Acenaphthene-d10	14.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetraethylene glycol	194	C8H18O5	000112-60-7	90
2	Pentaethylene glycol	238	C10H22O6	004792-15-8	83
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	78
4	3,6,9,12-Tetraoxatetradecan-1-ol	222	C10H22O5	005650-20-4	78
5	Triethylene glycol	150	C6H14O4	000112-27-6	74





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Sample : M3775-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PE-3

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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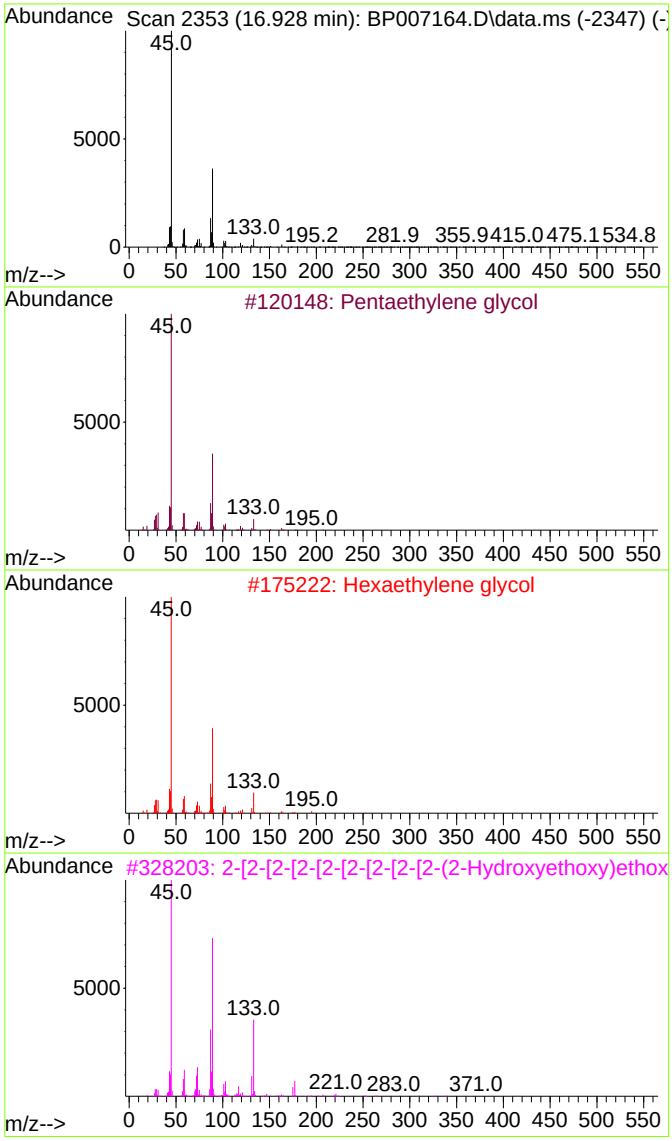
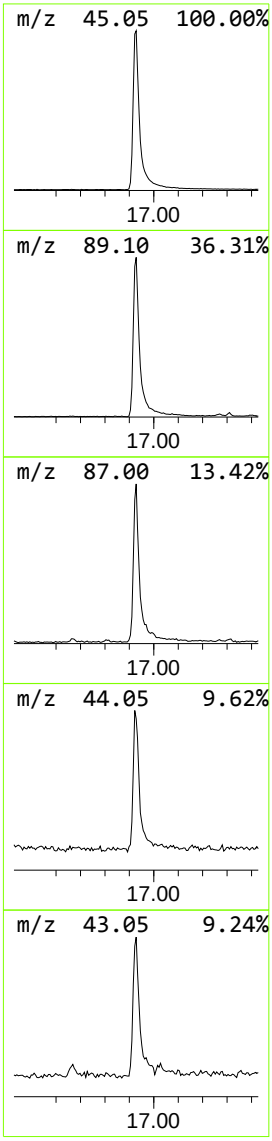
Peak Number 6 Pentaethylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.928	6.12 ng	971470	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	91
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	86
3	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	005579-66-8	83
4	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	78
5	3,6,9,12-Tetraoxatetradecan-1-ol	222	C10H22O5	005650-20-4	78





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Sample : M3775-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PE-3

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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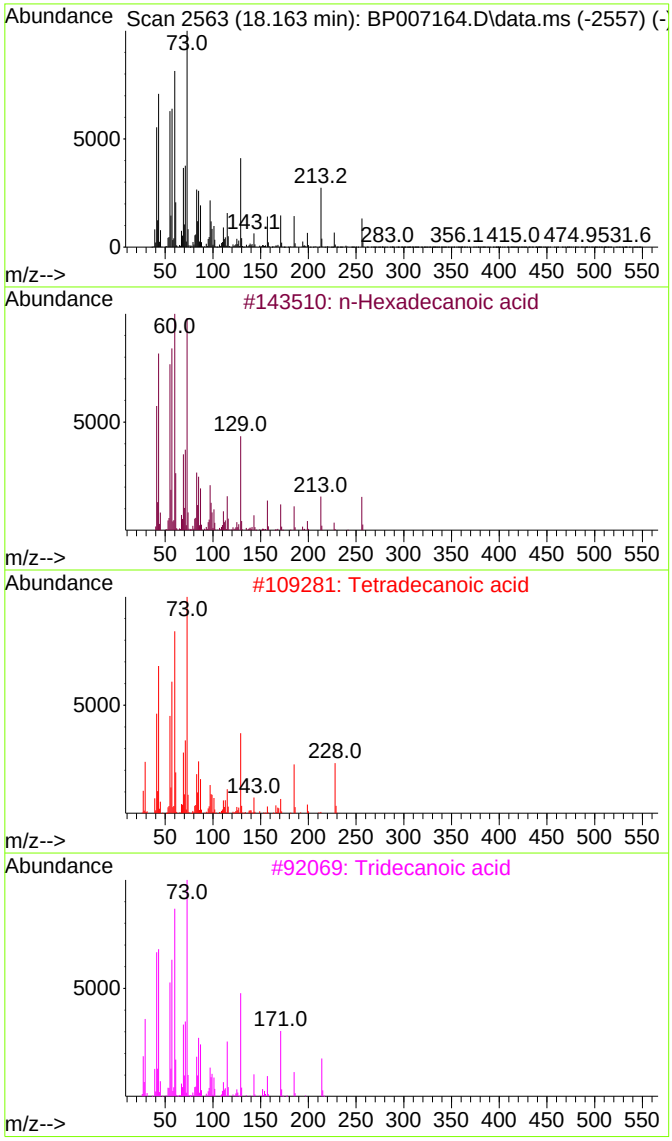
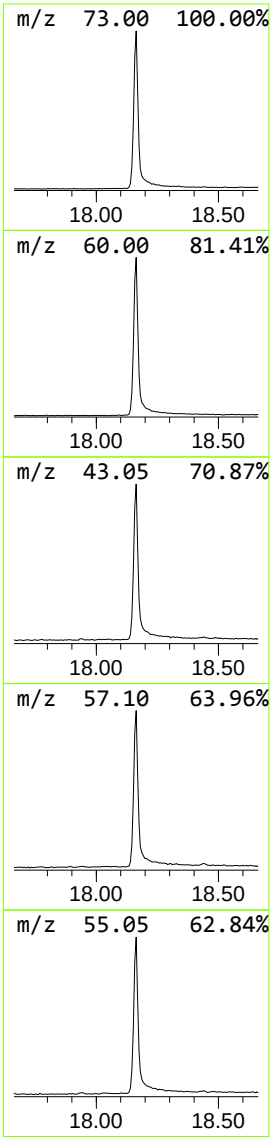
Peak Number 7 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.163	21.61 ng	3431450	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	Tridecanoic acid	214	C13H26O2	000638-53-9	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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TIC Library : C:\Database\NIST20.L
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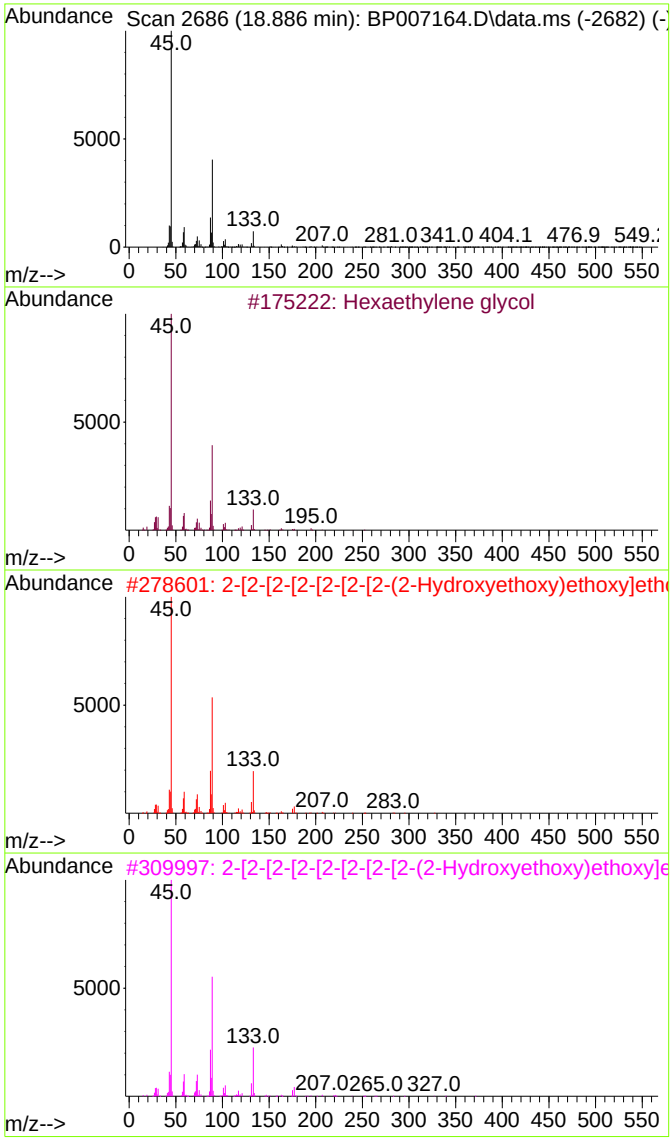
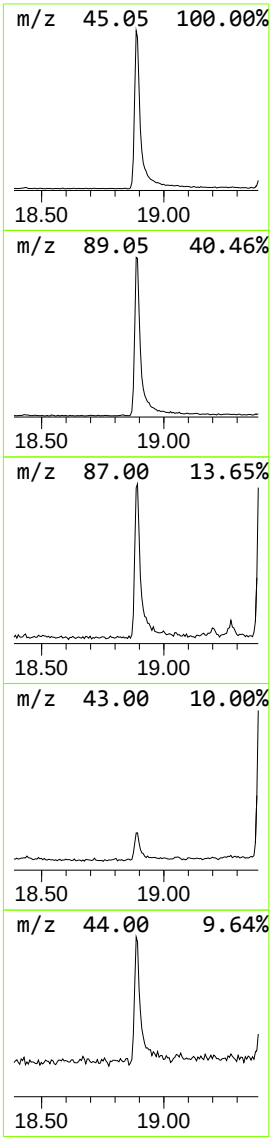
Peak Number 8 Hexaethylene glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.886	4.12 ng	653799	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	91
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	90
3	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	83
4	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	005579-66-8	83
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	83





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Operator : CG/JU
Sample : M3775-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PE-3

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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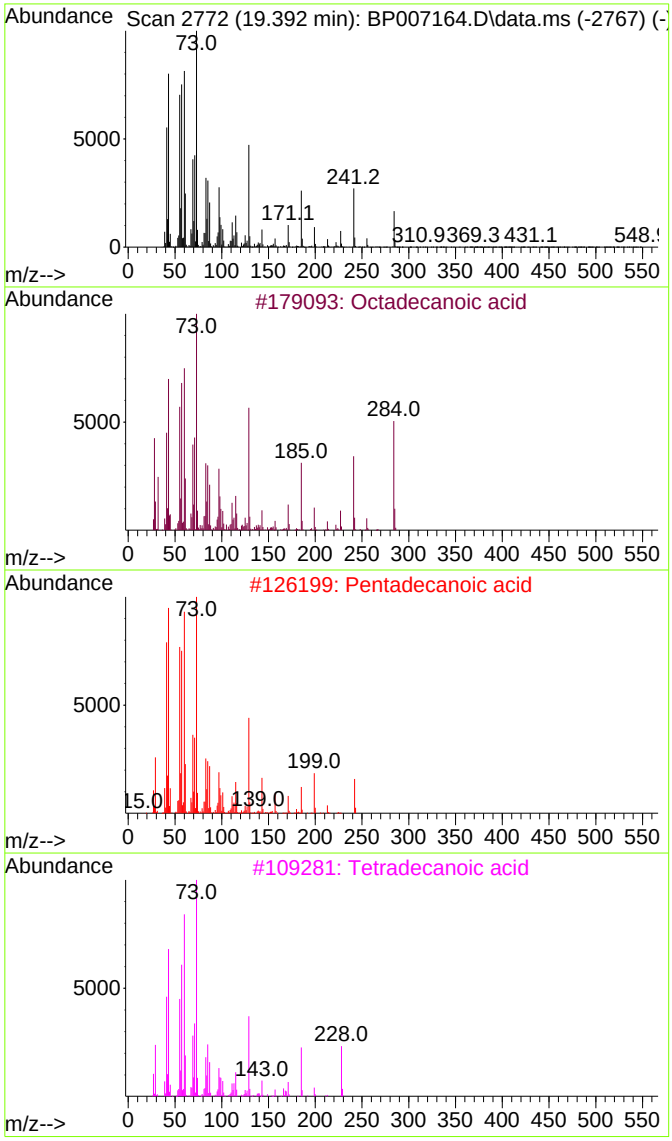
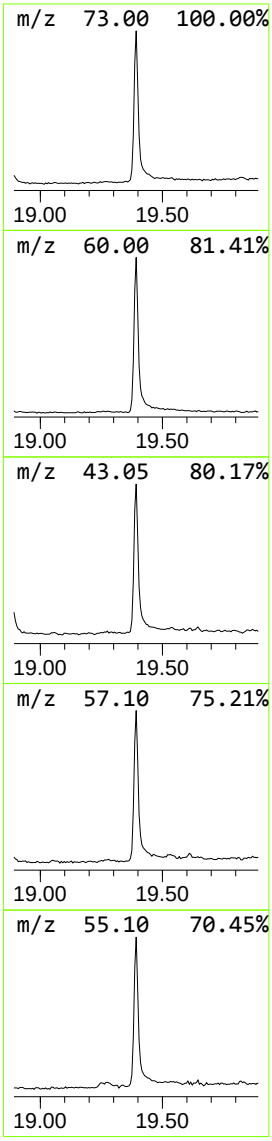
Peak Number 9 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.392	9.49 ng	1728420	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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Data File : BP007164.D
Acq On : 24 Sep 2021 18:15
Operator : CG/JU
Sample : M3775-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PE-3

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

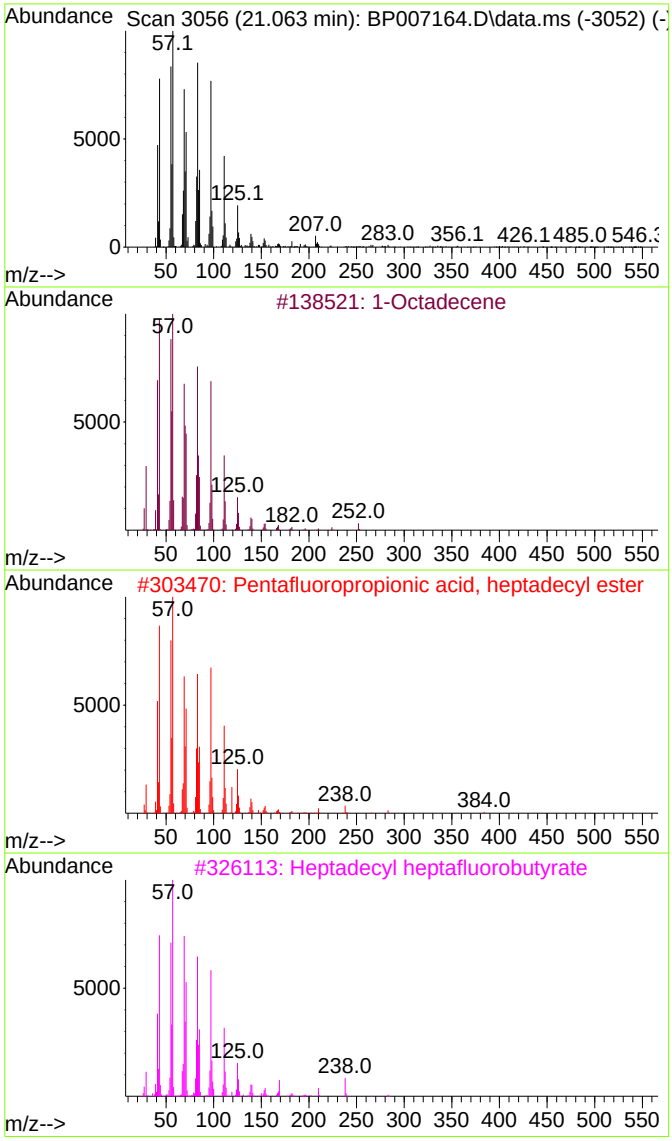
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

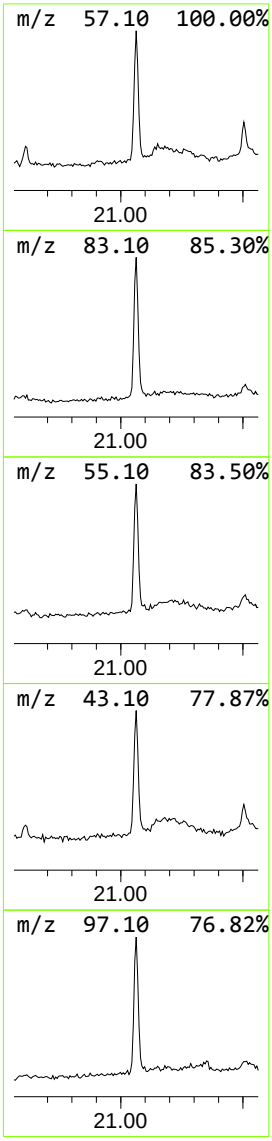
****

Peak Number 10 1-Octadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	3.79 ng	690288	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	94
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007164.D
Acq On : 24 Sep 2021 18:15
Operator : CG/JU
Sample : M3775-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PE-3

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.999	6.3	ng	443491	1	7.887	1402580	20.0
Ethanol, 2-(2-b...	10.469	2.9	ng	292798	2	10.687	1993900	20.0
Triethylene glycol	11.034	3.2	ng	322893	2	10.687	1993900	20.0
D-Allose	14.387	7.4	ng	1048340	3	14.516	2828710	20.0
Tetraethylene g...	14.440	8.4	ng	1185090	3	14.516	2828710	20.0
Pentaethylene g...	16.928	6.1	ng	971470	4	17.269	3175700	20.0
n-Hexadecanoic ...	18.163	21.6	ng	3431450	4	17.269	3175700	20.0
Hexaethylene gl...	18.886	4.1	ng	653799	4	17.269	3175700	20.0
Octadecanoic acid	19.392	9.5	ng	1728420	5	21.351	3643950	20.0
1-Octadecene	21.063	3.8	ng	690288	5	21.351	3643950	20.0