LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

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-BP091621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007028.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	322	328	338	rBV	183584	268084	1.33%	0.294%
2	5.475	400	406	420	rBV	2288899	3347980	16.56%	3.667%
3	7.069	668	677	687	rBV	1357599	2103708	10.41%	2.304%
4	7.910	808	820	829	rBV	1038021	1712133	8.47%	1.875%
5	9.069	1009	1017	1028	rBV	2989903	4887206	24.18%	5.353%
6	10.493	1253	1259	1269	rBV	186934	342027	1.69%	0.375%
7	10.710	1287	1296	1301	rBV	1391876	2390880	11.83%	2.619%
8	13.163	1704	1713	1724	rBV	8367005	12410494	61.39%	13.594%
9	14.534	1936	1946	1954	rBV	2305953	3311274	16.38%	3.627%
10	14.951	2010	2017	2030	rBV	263507	523720	2.59%	0.574%
11	16.022	2192	2199	2212	rBV	6809680	9791343	48.44%	10.725%
12	16.204	2224	2230	2236	rBV	522279	793649	3.93%	0.869%
13	17.281	2407	2413	2419	rBV	2946943	4039278	19.98%	4.424%
14	18.175	2557	2565	2590	rBV	4063102	6854937	33.91%	7.509%
15	18.480	2613	2617	2623	rVB2	149010	233291	1.15%	0.256%
16	19.222	2735	2743	2747	rBV	241155	630212	3.12%	0.690%
17	19.327	2755	2761	2767	rVB	340137	735271	3.64%	0.805%
18	19.404	2767	2774	2791	rBV	3388309	5946430	29.42%	6.513%
19	19.839	2842	2848	2853	rBV	16140695	20214329	100.00%	22.142%
20	20.616	2976	2980	2985	rBV2	131458	211413	1.05%	0.232%
21	21.074	3054	3058	3064	rBV2	518188	681469	3.37%	0.746%
22	21.357	3101	3106	3112	rBV	3657299	4816677	23.83%	5.276%
23	23.774	3510	3517	3528	rVB2	2326179	5048583	24.98%	5.530%

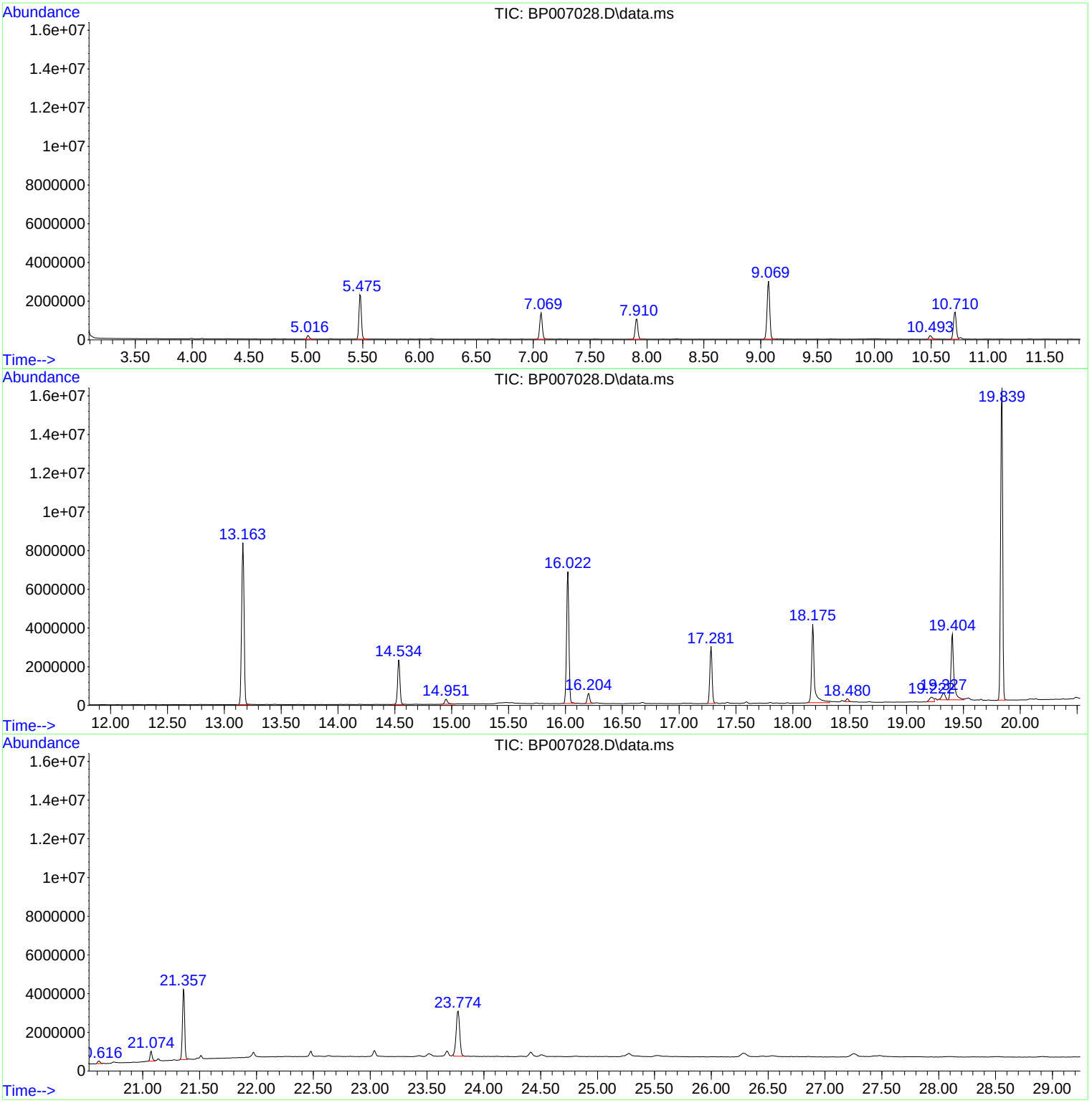
Sum of corrected areas: 91294388

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.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\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

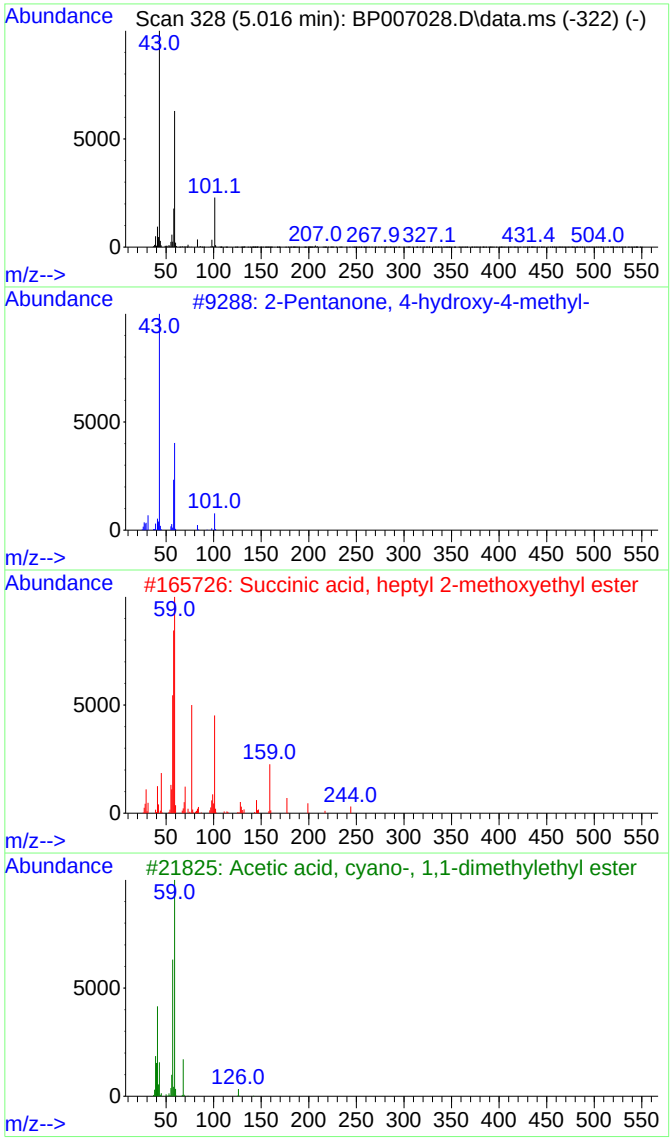
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

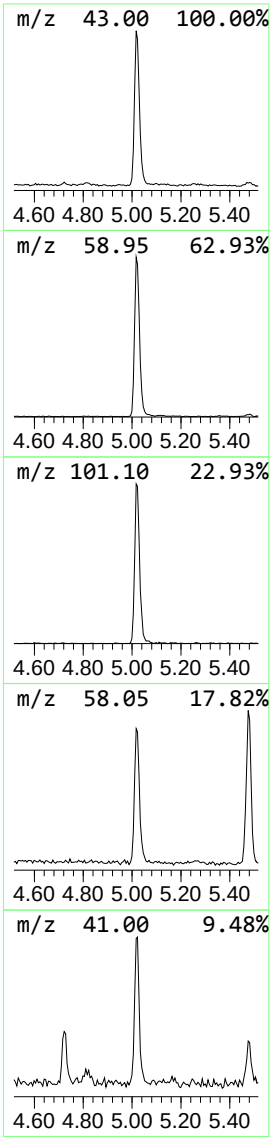
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	3.13 ng	268084	1,4-Dichlorobenzene-d4	7.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
5	Tetraglyme	222	C10H22O5	000143-24-8	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

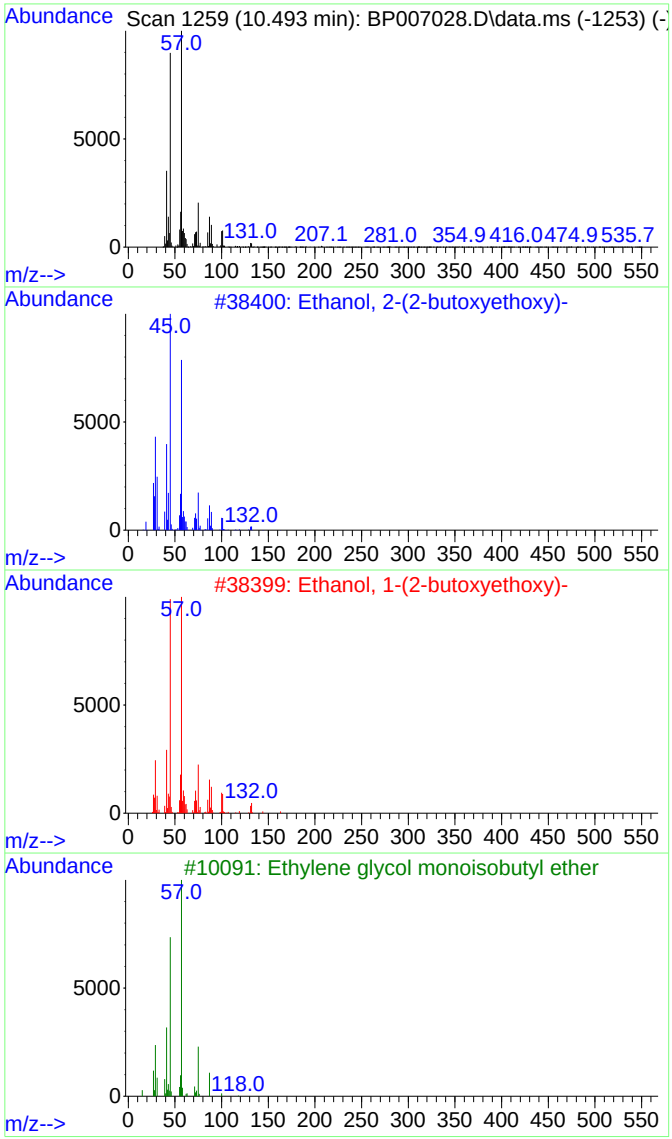
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

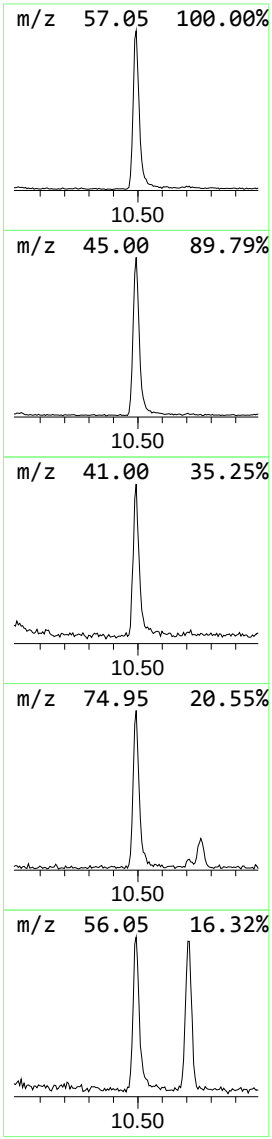
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.493	2.86 ng	342027	Naphthalene-d8	10.710

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	78
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

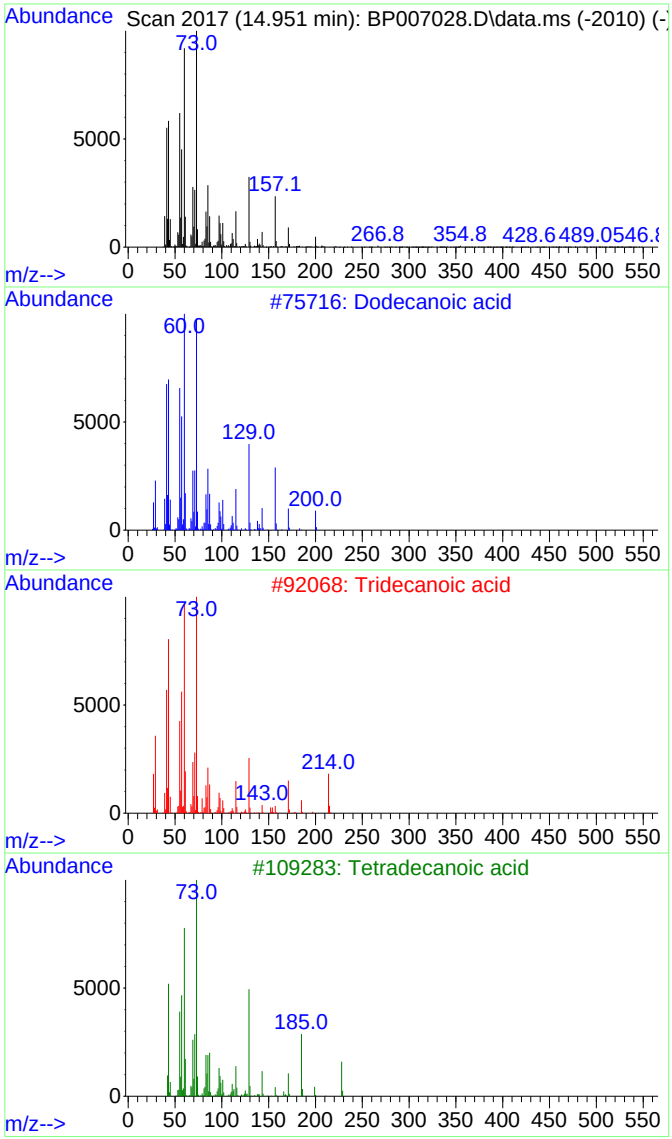
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

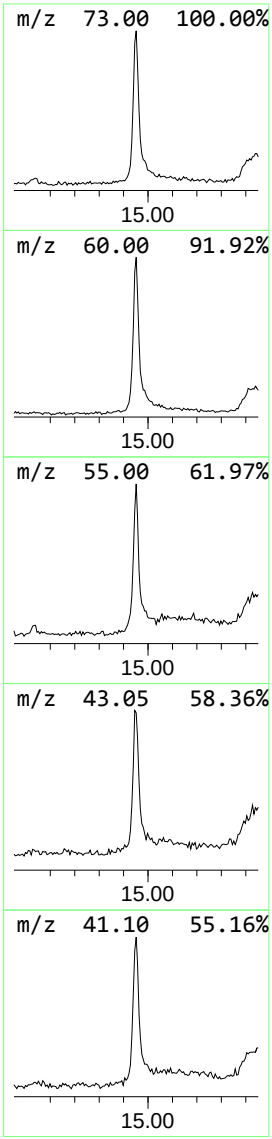
****

Peak Number 3 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.951	3.16 ng	523720	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Nonanoic acid	158	C9H18O2	000112-05-0	62
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

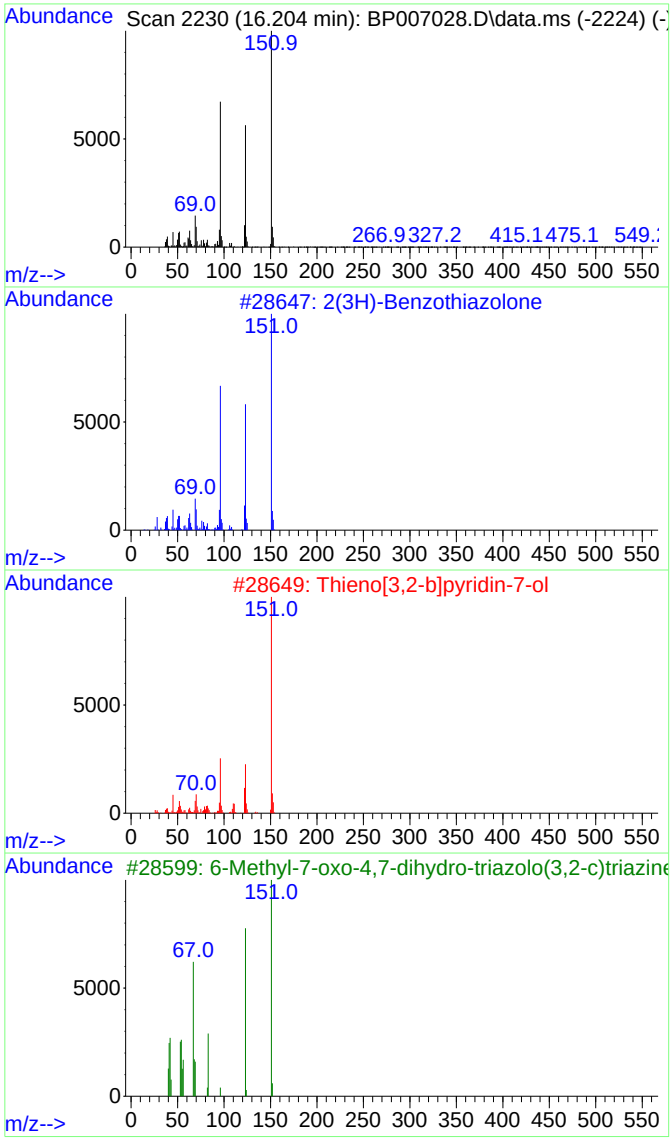
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

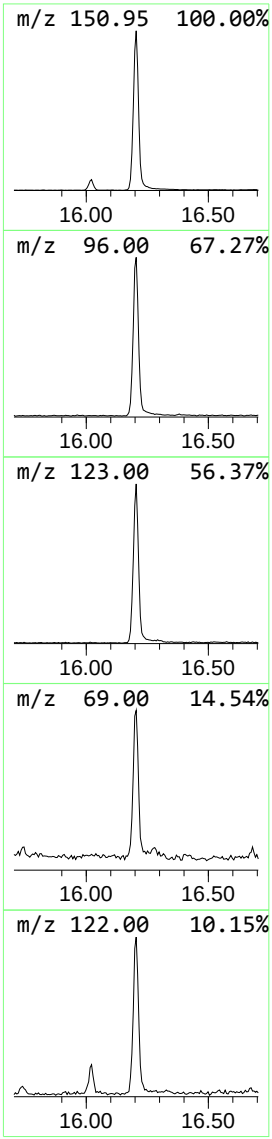
****

Peak Number 4 2(3H)-Benzothiazolone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.204	3.93 ng	793649	Phenanthrene-d10	17.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	96
2	Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	64
3	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	50
4	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	50
5	2-Mercapto-1,3-benzoxazole	151	C7H5NOS	002382-96-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

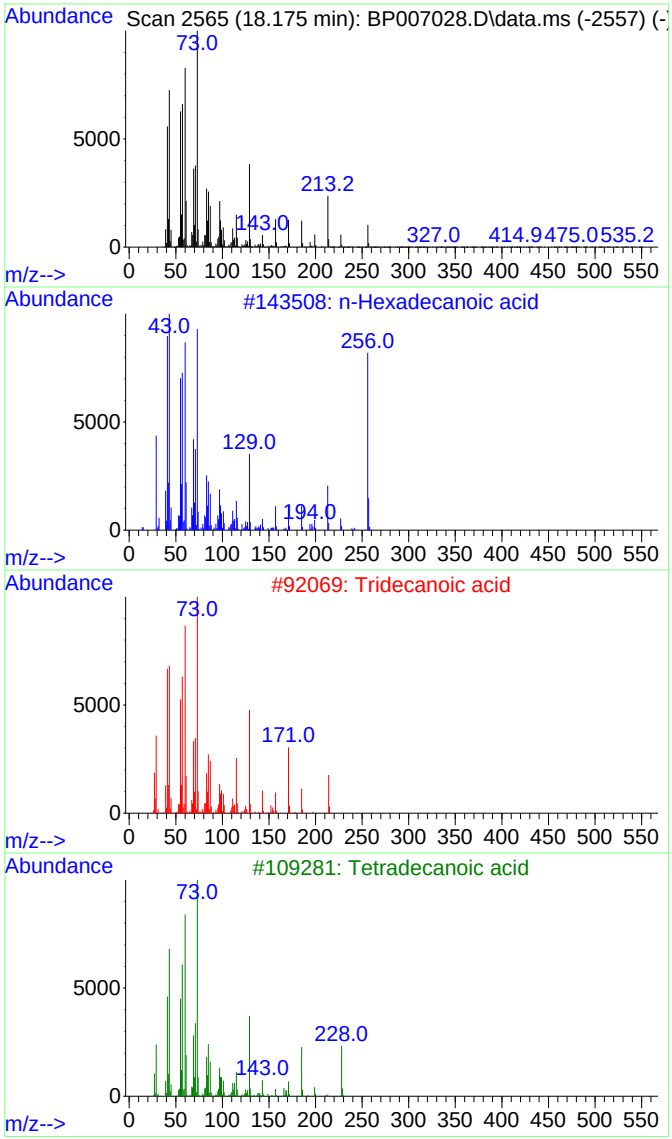
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

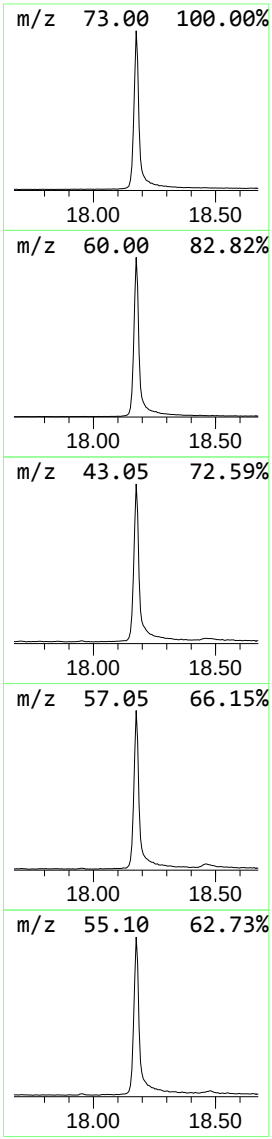
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.175	33.94 ng	6854940	Phenanthrene-d10	17.281

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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

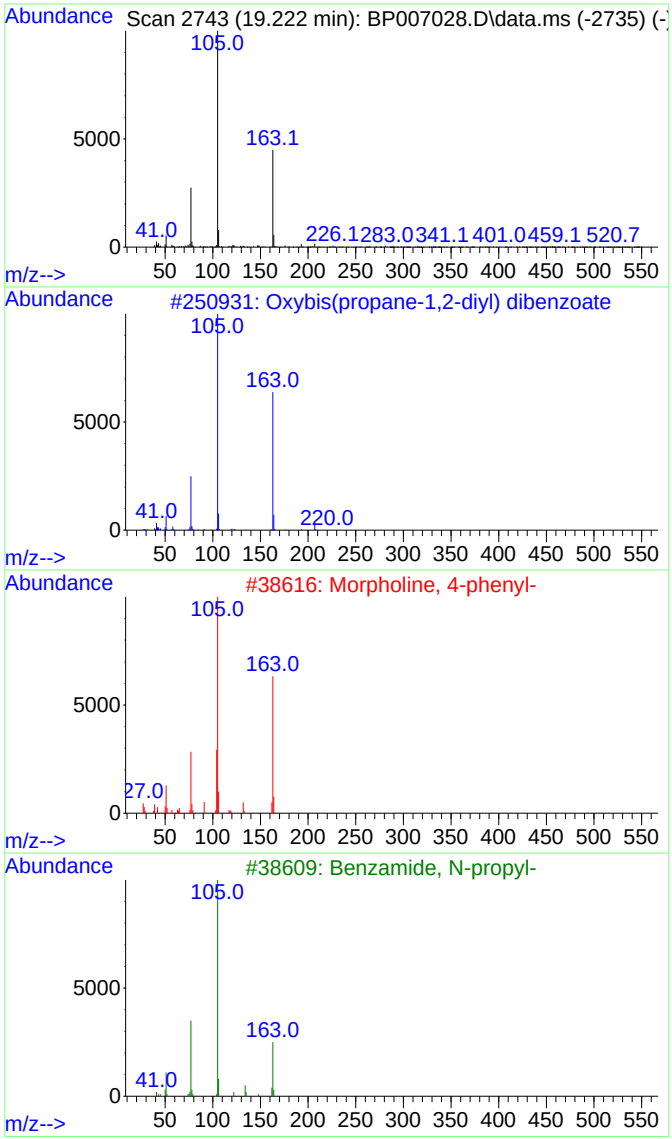
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

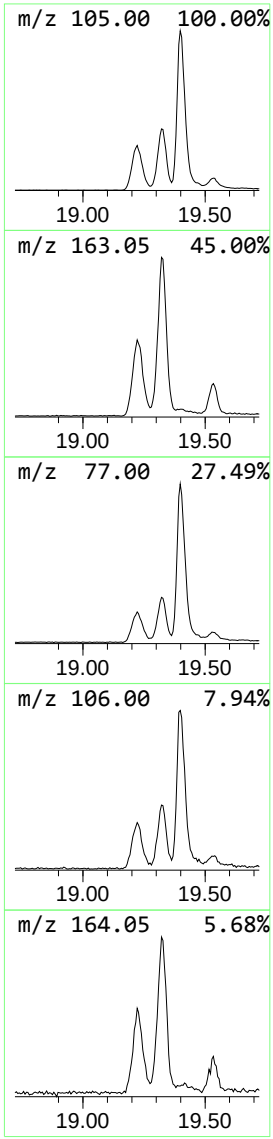
****

Peak Number 6 Oxybis(propane-1,2-diyl) di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.222	3.12 ng	630212	Phenanthrene-d10	17.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	78
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
3	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	43
4	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	36
5	Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

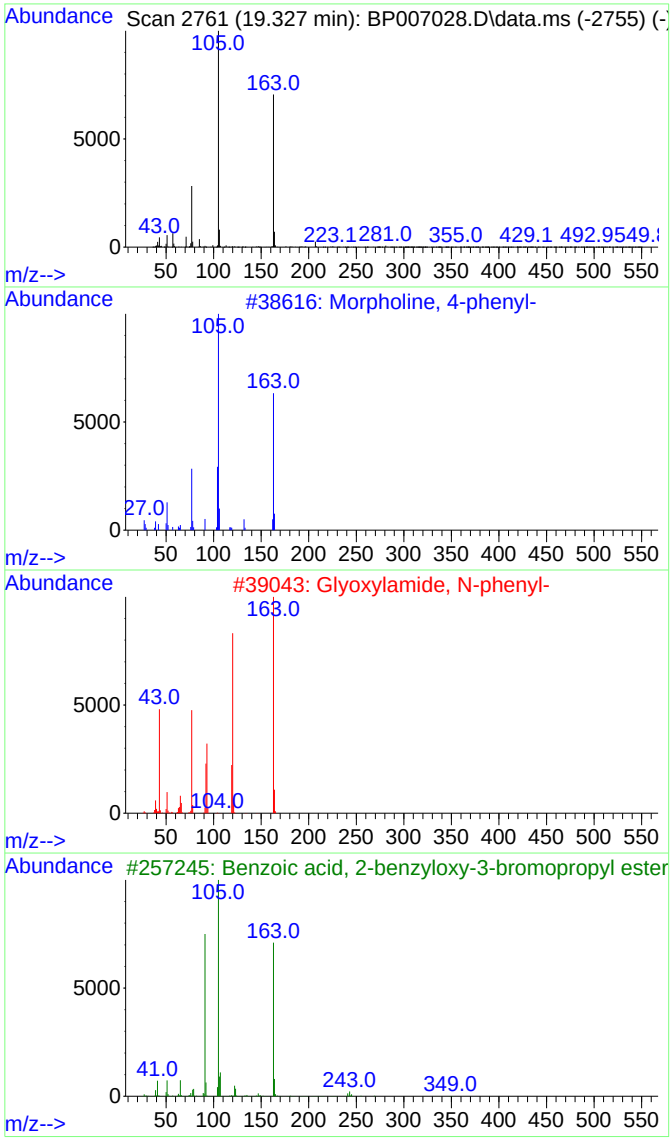
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

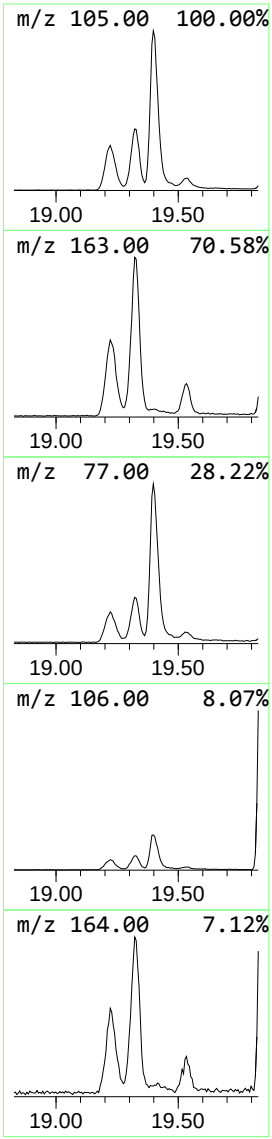
****

Peak Number 7 Morpholine, 4-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.328	3.05 ng	735271	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
3	Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	40
4	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	38
5	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

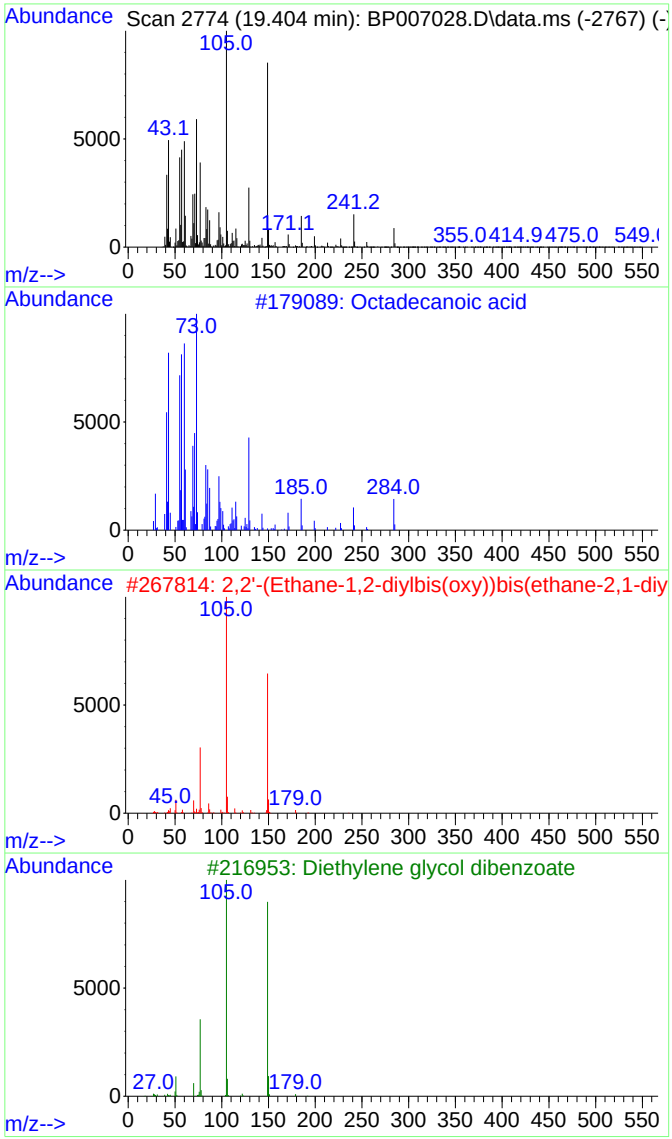
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

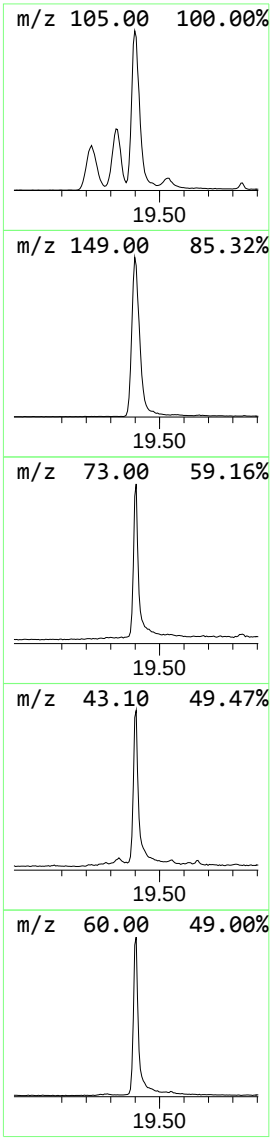
****

Peak Number 8 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	24.69 ng	5946430	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	46
3	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	46
4	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	38
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

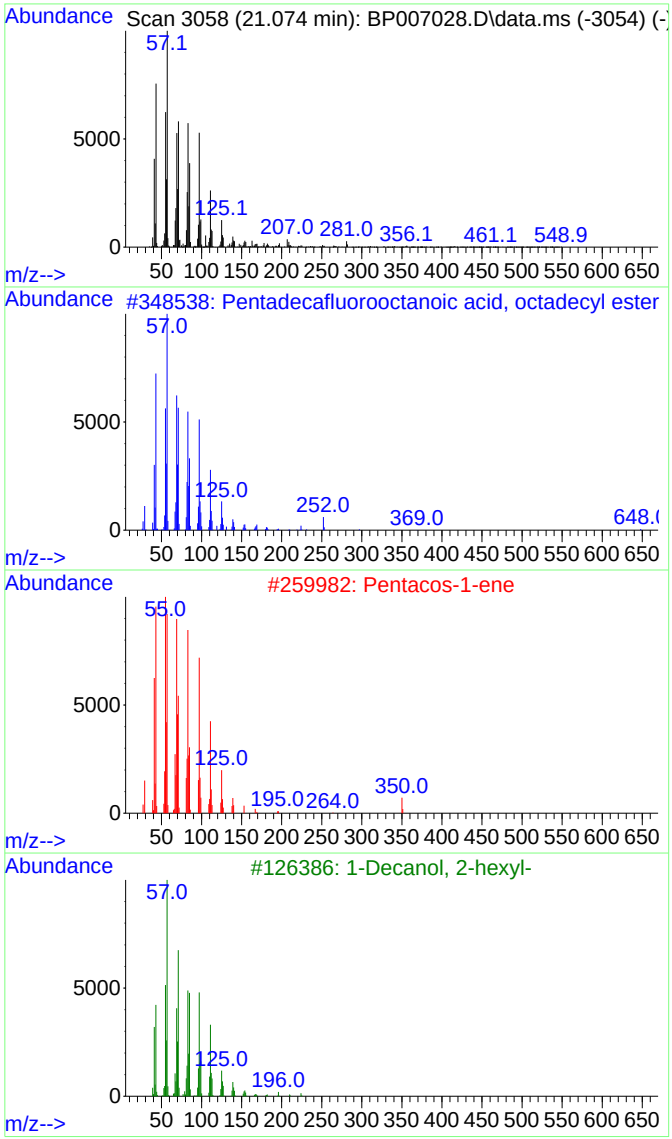
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

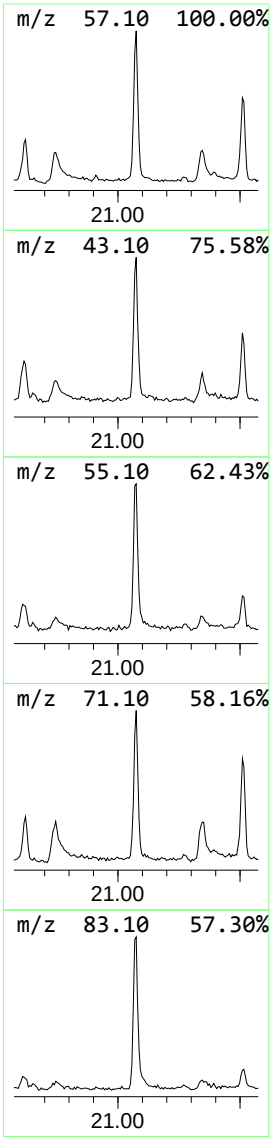
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pentadecafluorooctanoic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.075	2.83 ng	681469	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Pentacos-1-ene	350	C25H50	016980-85-1	93
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
4	Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	90
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007028.D
Acq On : 17 Sep 2021 16:13
Operator : CG/JU
Sample : M3774-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-RR-02-(1.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.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-...	5.016	3.1	ng	268084	1	7.910	1712130	20.0
Ethanol, 2-(2-b...	10.493	2.9	ng	342027	2	10.710	2390880	20.0
Dodecanoic acid	14.951	3.2	ng	523720	3	14.534	3311270	20.0
2(3H)-Benzothia...	16.204	3.9	ng	793649	4	17.281	4039280	20.0
n-Hexadecanoic ...	18.175	33.9	ng	6854940	4	17.281	4039280	20.0
Oxybis(propane-...	19.222	3.1	ng	630212	4	17.281	4039280	20.0
Morpholine, 4-p...	19.328	3.0	ng	735271	5	21.357	4816680	20.0
Octadecanoic acid	19.404	24.7	ng	5946430	5	21.357	4816680	20.0
Pentadecafluoro...	21.075	2.8	ng	681469	5	21.357	4816680	20.0