LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120221\
Data File : BP008196.D
Acq On : 02 Dec 2021 17:44
Operator : CG/JU
Sample : M4891-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MINEBROOK-2-COMP

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-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008196.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.046	8	10	20	rVB	55752	62954	1.03%	0.212%
2	4.923	323	329	342	rBV	481107	669872	10.99%	2.252%
3	5.387	400	408	422	rBV	2119454	3069664	50.38%	10.320%
4	6.981	670	679	694	rBV	1925702	3175963	52.13%	10.678%
5	7.793	808	817	826	rBV	370839	582822	9.57%	1.959%
6	8.958	1006	1015	1032	rBV	1252560	2100178	34.47%	7.061%
7	10.393	1252	1259	1268	rBV	32592	76446	1.25%	0.257%
8	10.593	1286	1293	1302	rBV	433121	740850	12.16%	2.491%
9	13.063	1706	1713	1727	rBV	2741837	4117984	67.59%	13.845%
10	14.440	1940	1947	1967	rBV	601748	976402	16.03%	3.283%
11	15.275	2081	2089	2092	rBV2	27799	65530	1.08%	0.220%
12	15.940	2192	2202	2222	rBV	2148787	3446388	56.56%	11.587%
13	17.204	2410	2417	2427	rBV	814910	1217741	19.99%	4.094%
14	18.104	2565	2570	2578	rBV2	87781	134200	2.20%	0.451%
15	19.775	2848	2854	2862	rBV	4758663	6092862	100.00%	20.484%
16	21.022	3062	3066	3074	rBV	223054	349233	5.73%	1.174%
17	21.310	3110	3115	3125	rBV	1095278	1465419	24.05%	4.927%
18	23.704	3516	3522	3534	rVB2	664683	1399546	22.97%	4.705%

Sum of corrected areas: 29744054

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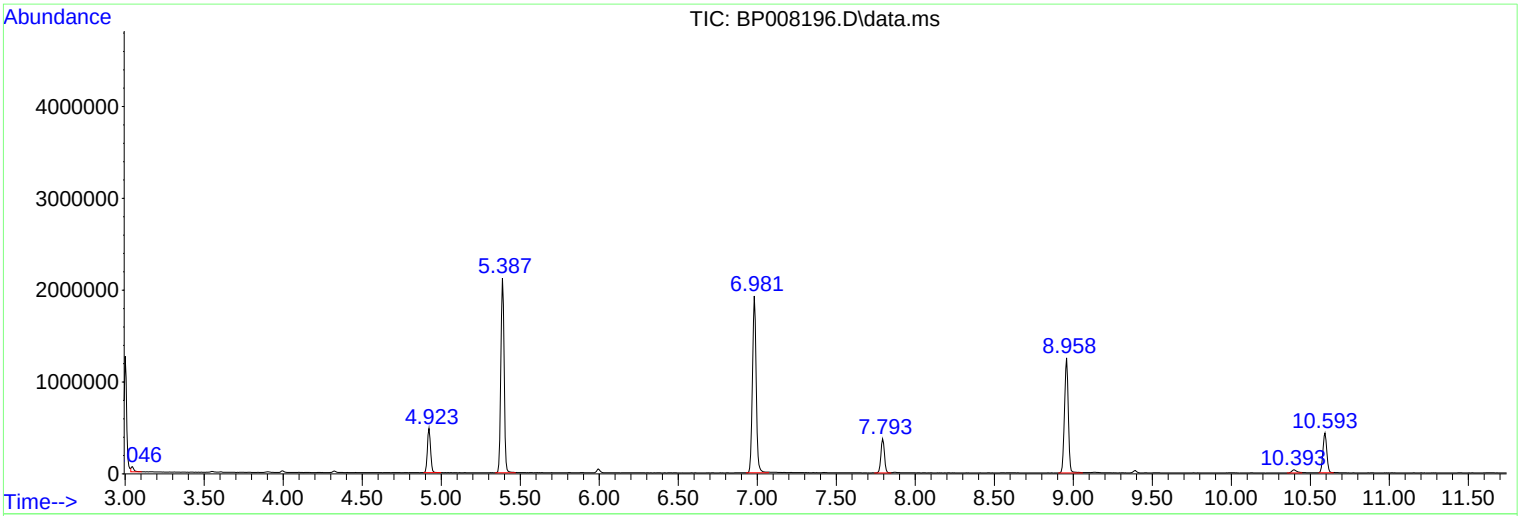
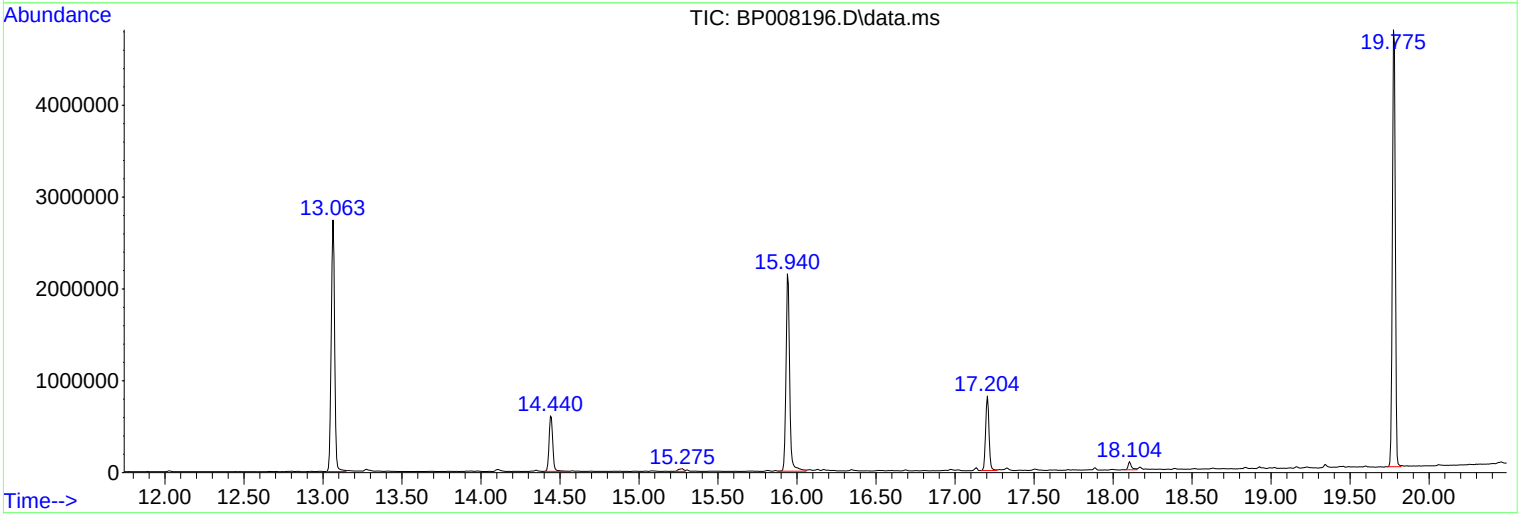
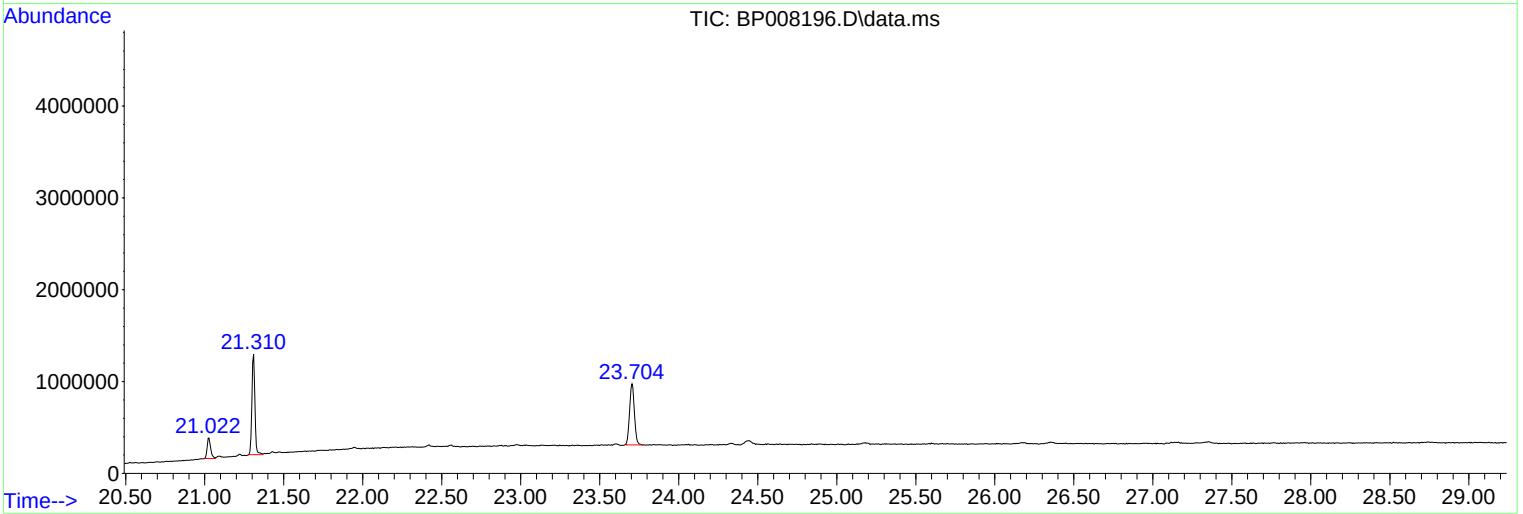
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

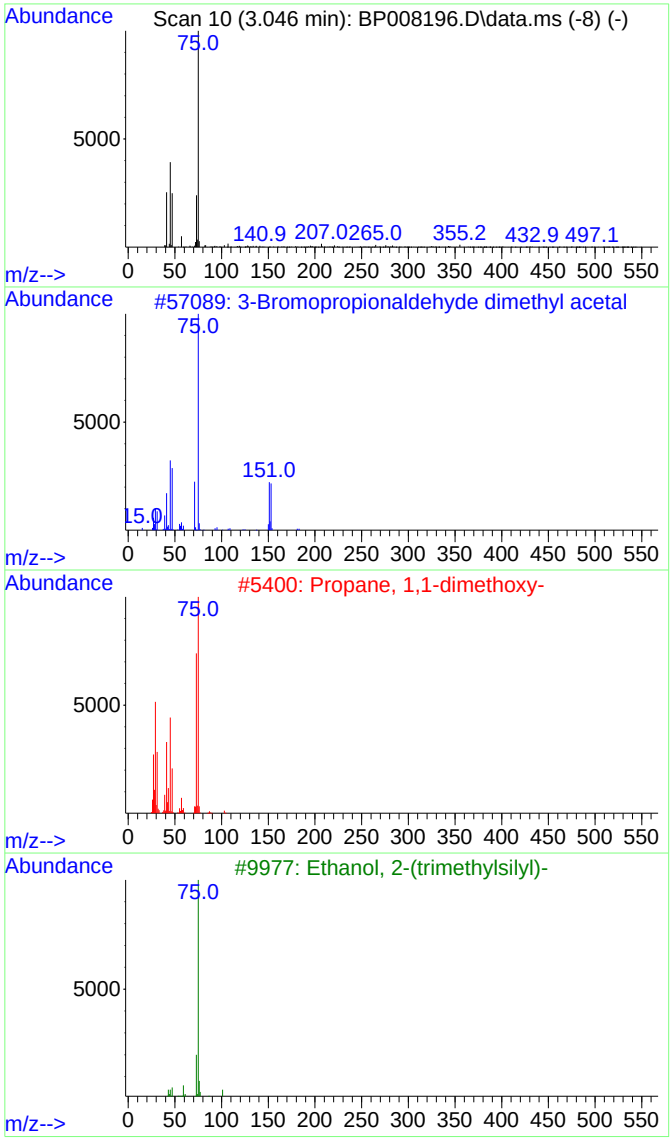
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

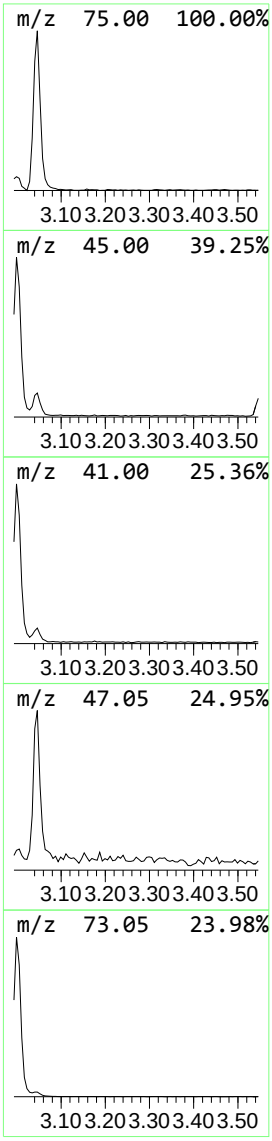
****

Peak Number 1 3-Bromopropionaldehyde dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.046	2.16 ng	62954	1,4-Dichlorobenzene-d4	7.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	64
2	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	38
3	Ethanol, 2-(trimethylsilyl)-	118	C5H14OSi	002916-68-9	9
4	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
5	benzene, 1-bromo-4-[(2,2-dimetho...	276	C10H13BrO2S	1000401-85-1	7





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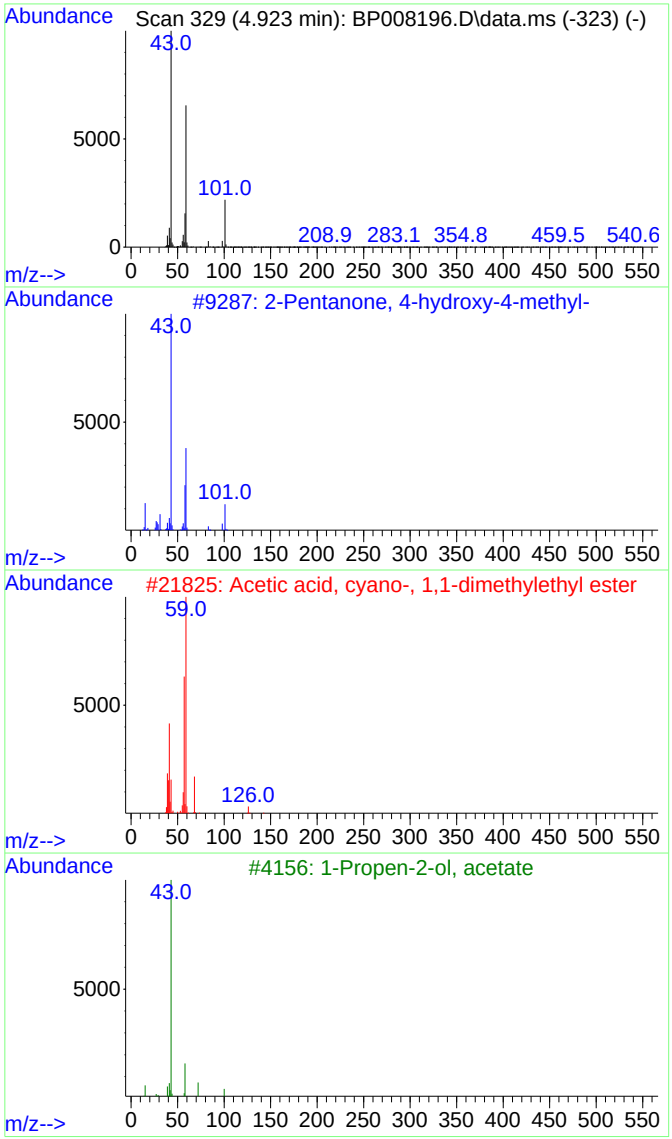
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

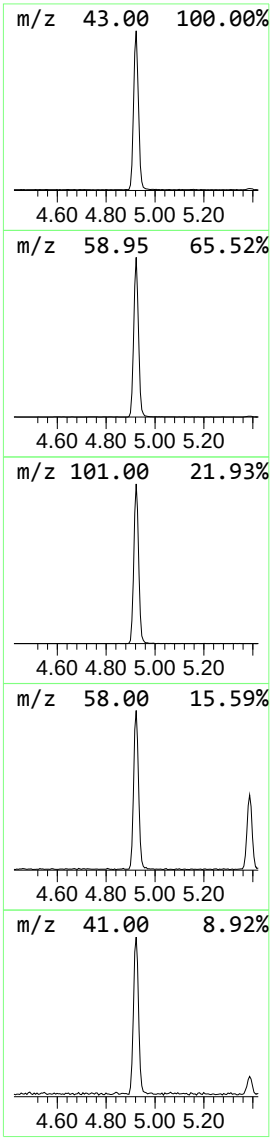
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.923	22.99 ng	669872	1,4-Dichlorobenzene-d4	7.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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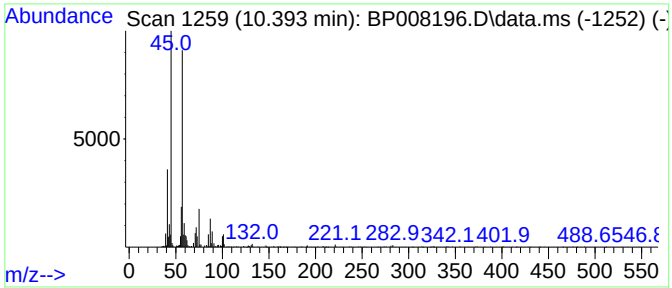
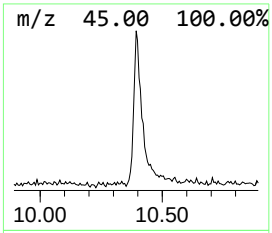
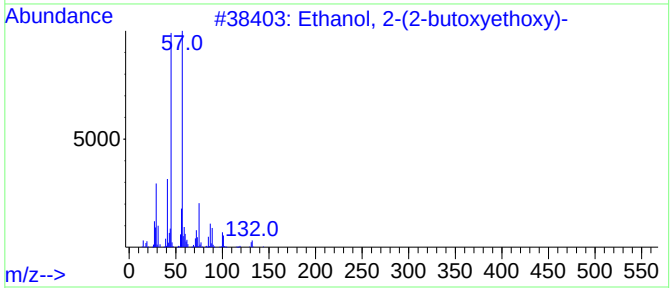
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

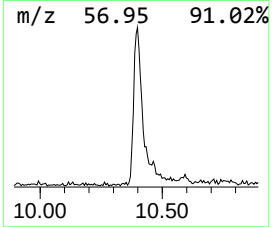
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.393	2.06 ng	76446	Naphthalene-d8	10.593

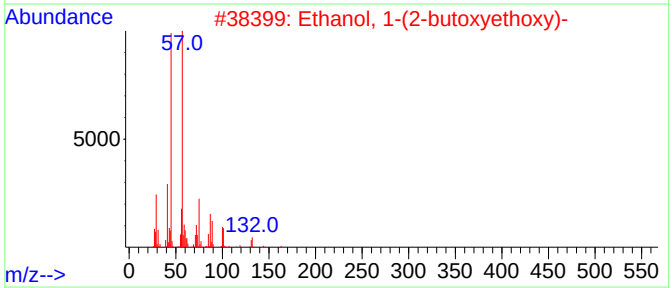
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	59
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53

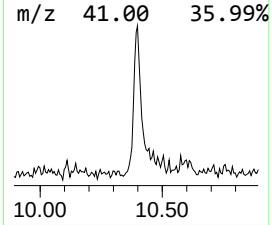


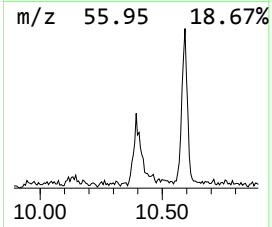


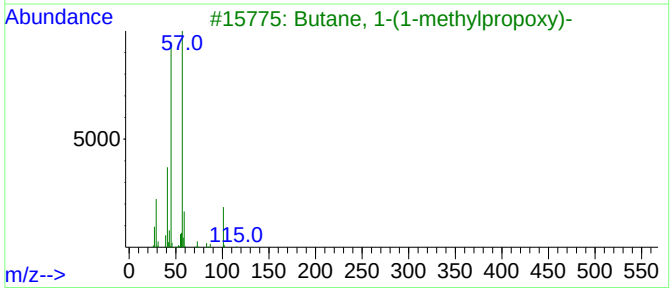


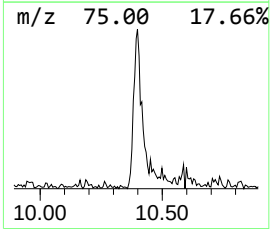












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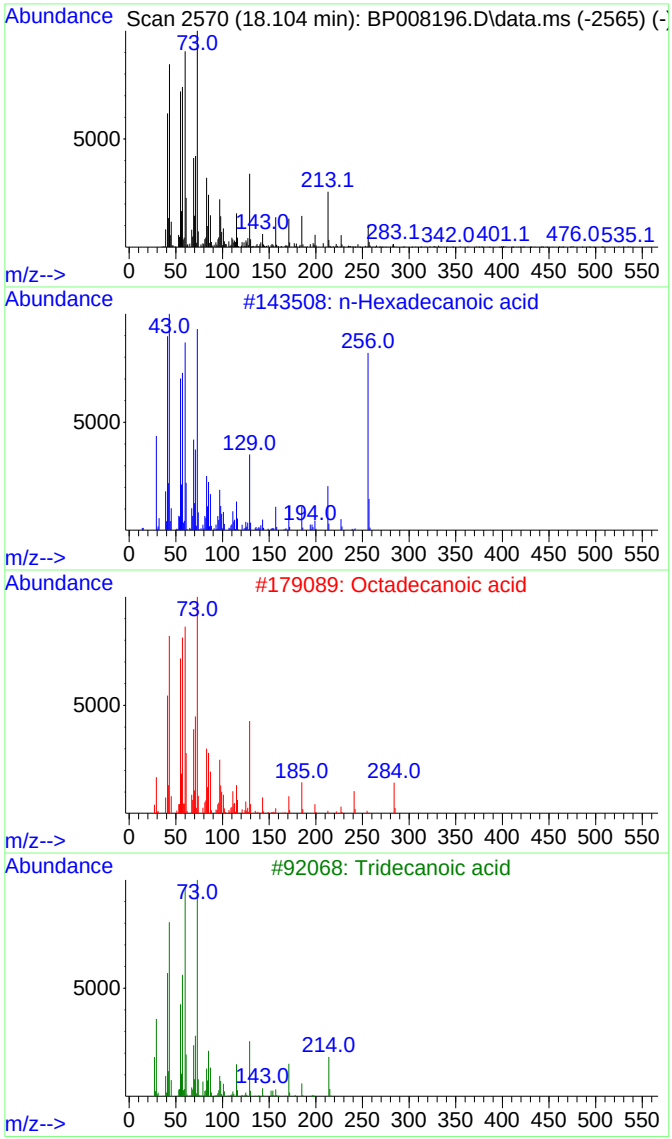
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

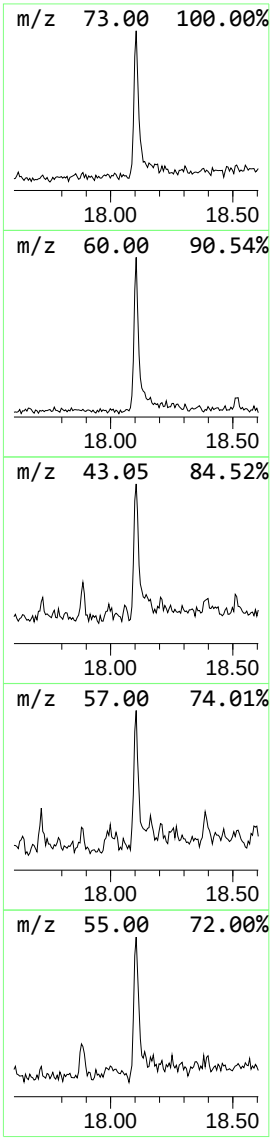
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	2.20 ng	134200	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





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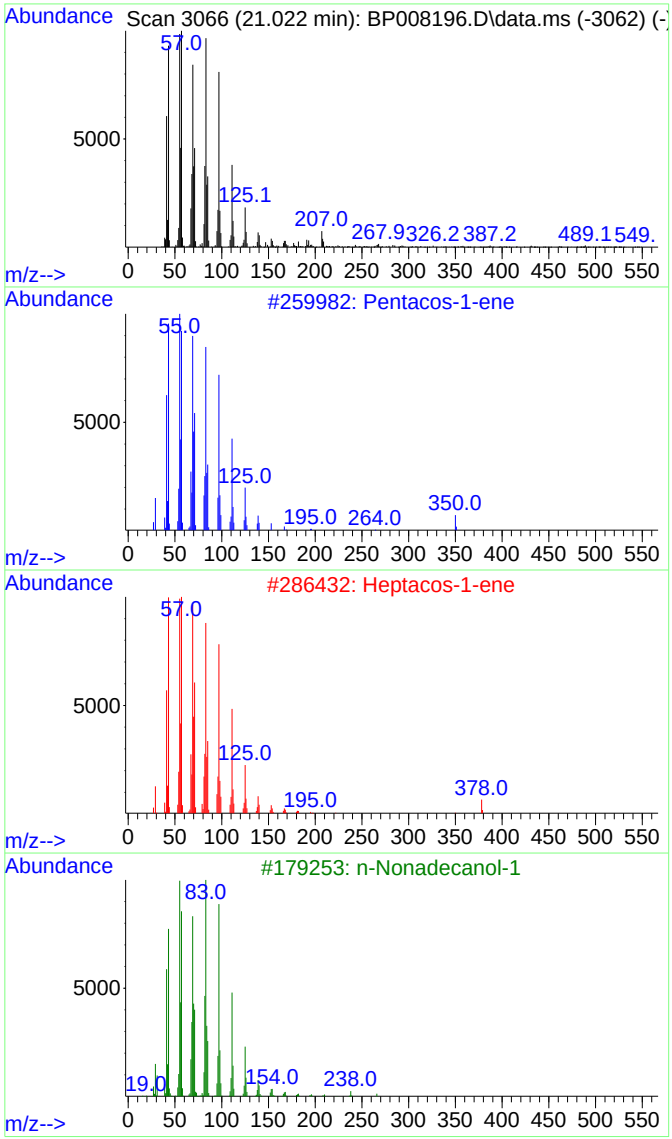
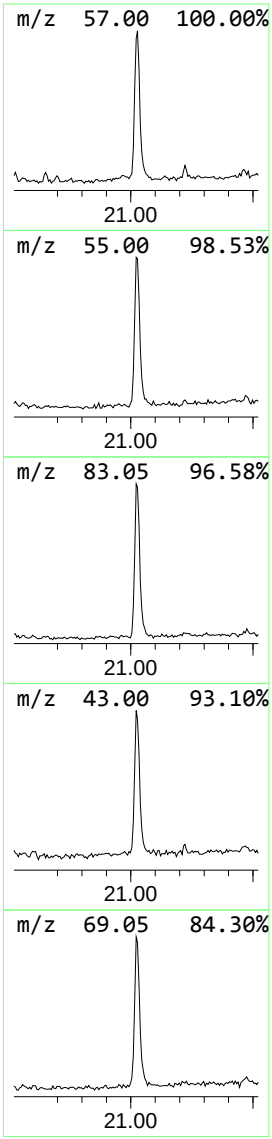
****

Peak Number 5 Pentacos-1-ene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.022	4.77 ng	349233	Chrysene-d12	21.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacos-1-ene	350	C25H50	016980-85-1	94
2	Heptacos-1-ene	378	C27H54	015306-27-1	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Bromopropiona...	3.046	2.2	ng	62954	1	7.793	582822	20.0
2-Pentanone, 4-...	4.923	23.0	ng	669872	1	7.793	582822	20.0
Ethanol, 2-(2-b...	10.393	2.1	ng	76446	2	10.593	740850	20.0
n-Hexadecanoic ...	18.104	2.2	ng	134200	4	17.204	1217740	20.0
Pentacos-1-ene	21.022	4.8	ng	349233	5	21.310	1465420	20.0