LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006535.D
Acq On : 06 Aug 2021 12:38
Operator : CG/JU
Sample : M3271-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-1

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-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006535.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.905	304	309	322	rVB	1056642	1452892	18.28%	2.842%
2	5.358	380	386	399	rVB	3261430	4536303	57.07%	8.875%
3	5.969	485	490	497	rVB	210609	300124	3.78%	0.587%
4	6.934	647	654	666	rBV	3131124	4787300	60.23%	9.366%
5	7.752	787	793	801	rVB	796992	1279552	16.10%	2.503%
6	8.910	982	990	1001	rBV	1962284	3139791	39.50%	6.143%
7	10.328	1224	1231	1242	rBV	276003	440583	5.54%	0.862%
8	10.540	1259	1267	1273	rBV	1066971	1792831	22.55%	3.507%
9	13.010	1679	1687	1697	rBV	4005321	5756162	72.41%	11.261%
10	14.381	1913	1920	1927	rBV	1478074	2226234	28.01%	4.355%
11	15.875	2164	2174	2194	rBV	3195071	4653091	58.54%	9.103%
12	17.133	2382	2388	2393	rBV	1744911	2538292	31.93%	4.966%
13	17.175	2393	2395	2401	rVV	313227	409698	5.15%	0.802%
14	17.269	2402	2411	2416	rVB2	55954	109805	1.38%	0.215%
15	18.045	2539	2543	2552	rBV2	528736	749474	9.43%	1.466%
16	18.192	2564	2568	2572	rBV2	56075	90383	1.14%	0.177%
17	19.151	2726	2731	2739	rBV	562498	750624	9.44%	1.468%
18	19.280	2749	2753	2761	rBV2	218953	329621	4.15%	0.645%
19	19.504	2783	2791	2800	rBV	506885	785325	9.88%	1.536%
20	19.716	2821	2827	2836	rVB	6282346	7948955	100.00%	15.551%
21	20.963	3035	3039	3044	rBV2	331767	424393	5.34%	0.830%
22	21.233	3079	3085	3089	rBV	2368300	3219332	40.50%	6.298%
23	21.269	3089	3091	3097	rVB	232254	270788	3.41%	0.530%
24	23.563	3475	3481	3498	rVB2	1513546	3123756	39.30%	6.111%

Sum of corrected areas: 51115309

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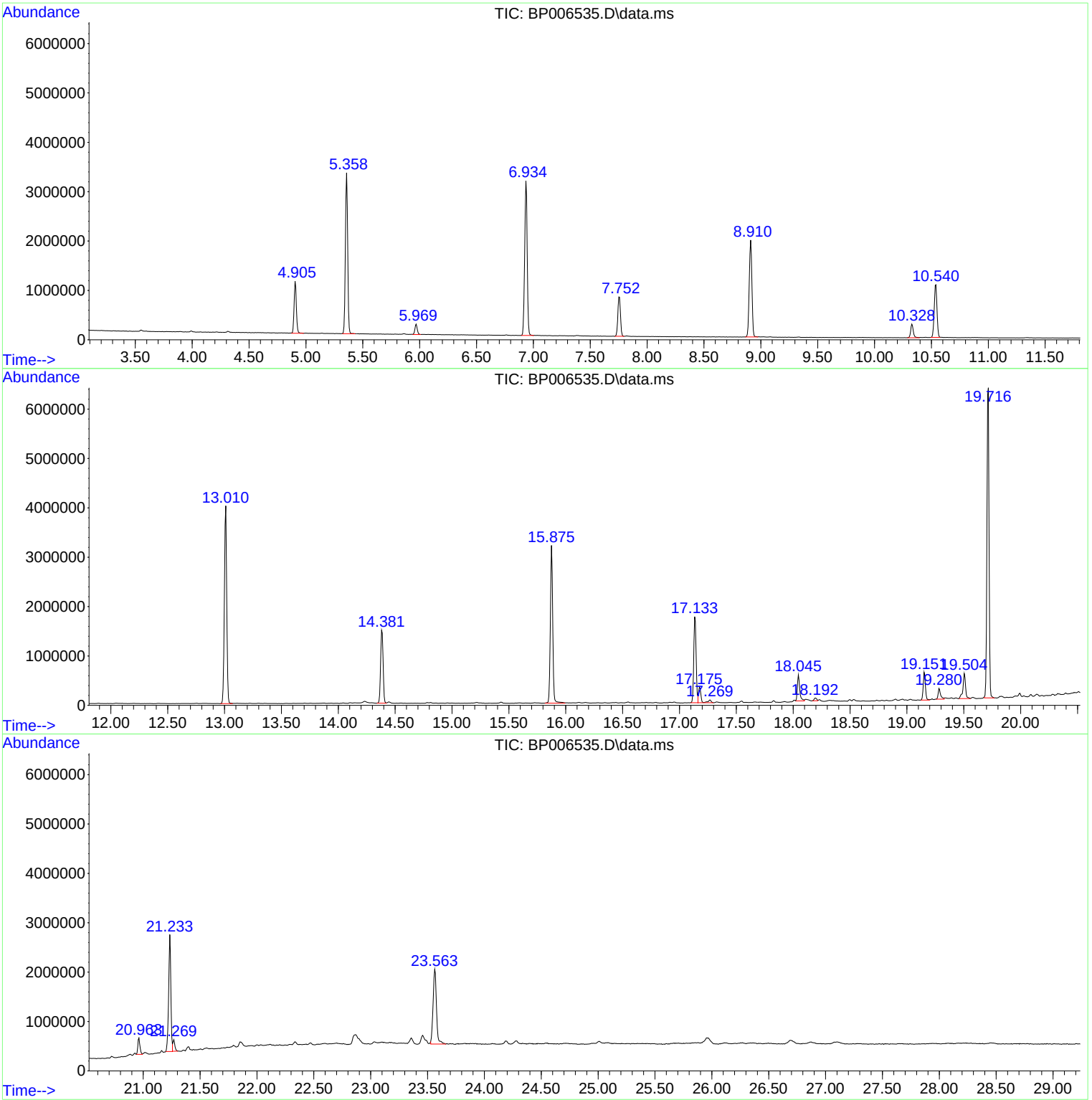
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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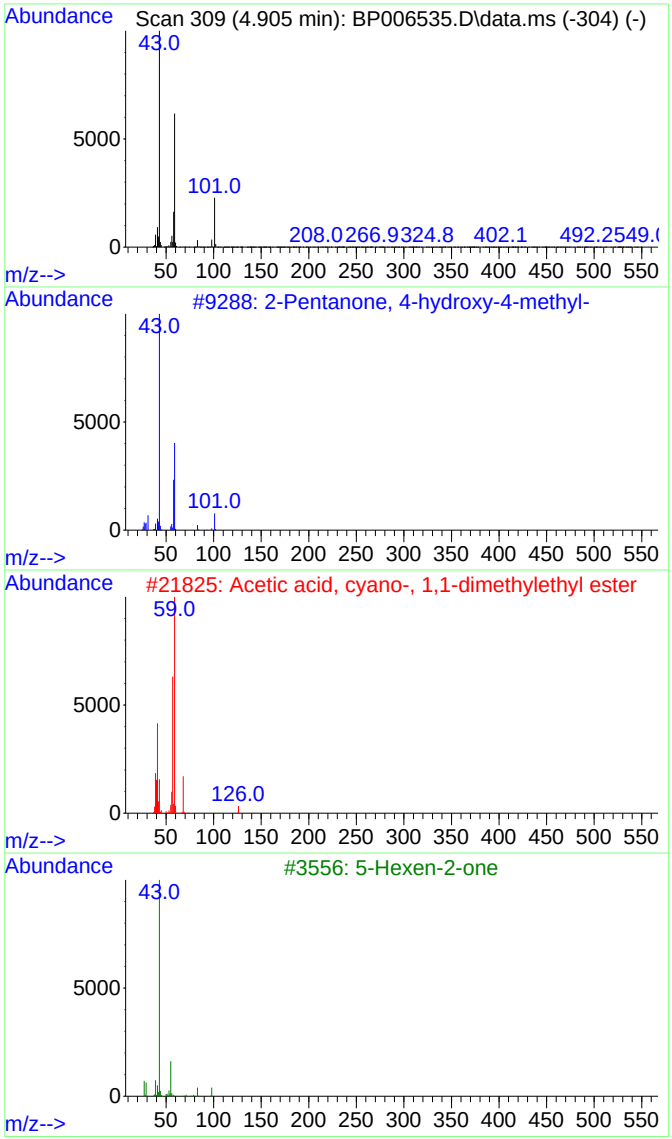
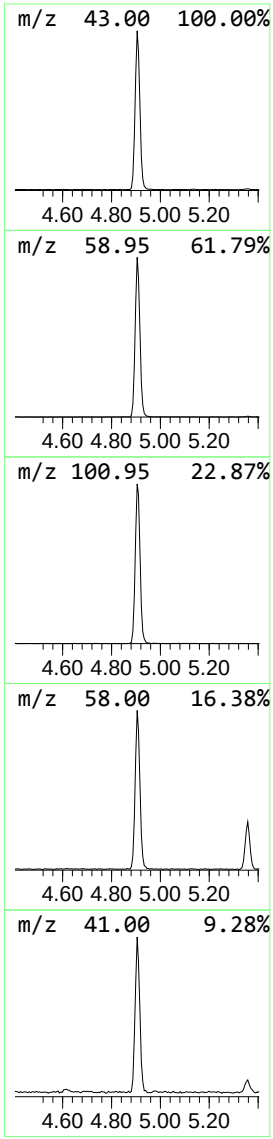
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	22.71 ng	1452890	1,4-Dichlorobenzene-d4	7.758

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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

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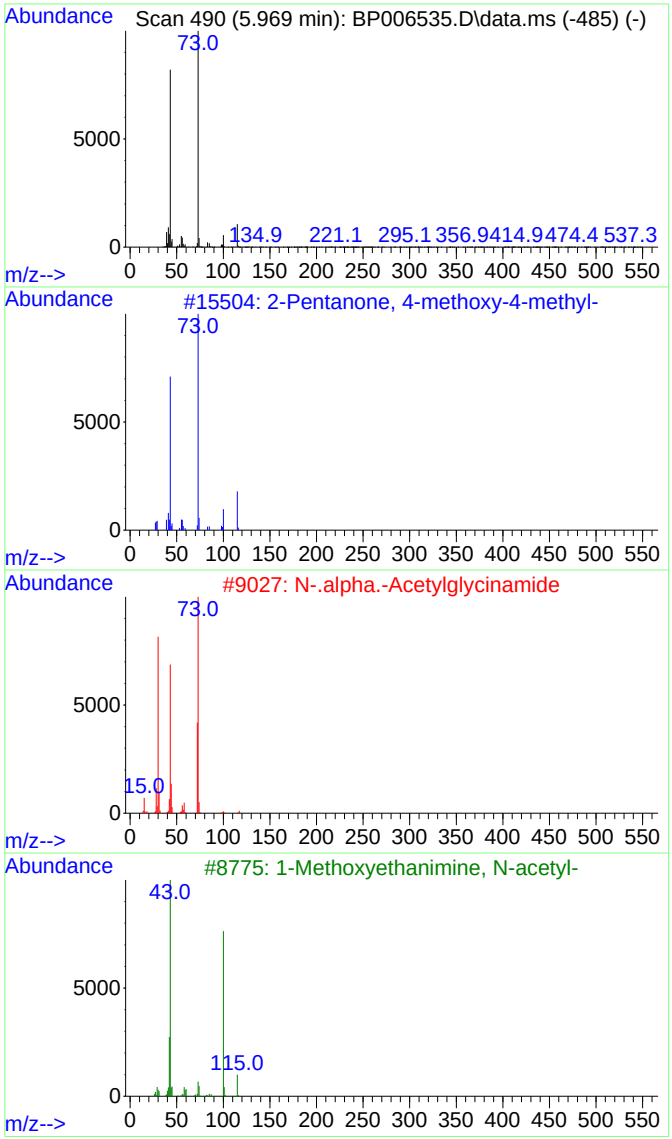
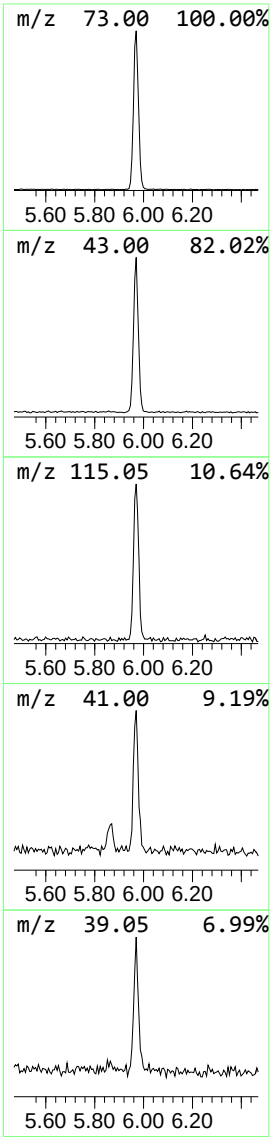
****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	4.69 ng	300124	1,4-Dichlorobenzene-d4	7.758

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	28
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Operator : CG/JU
Sample : M3271-01
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Instrument :
BNA_P
ClientSampleId :
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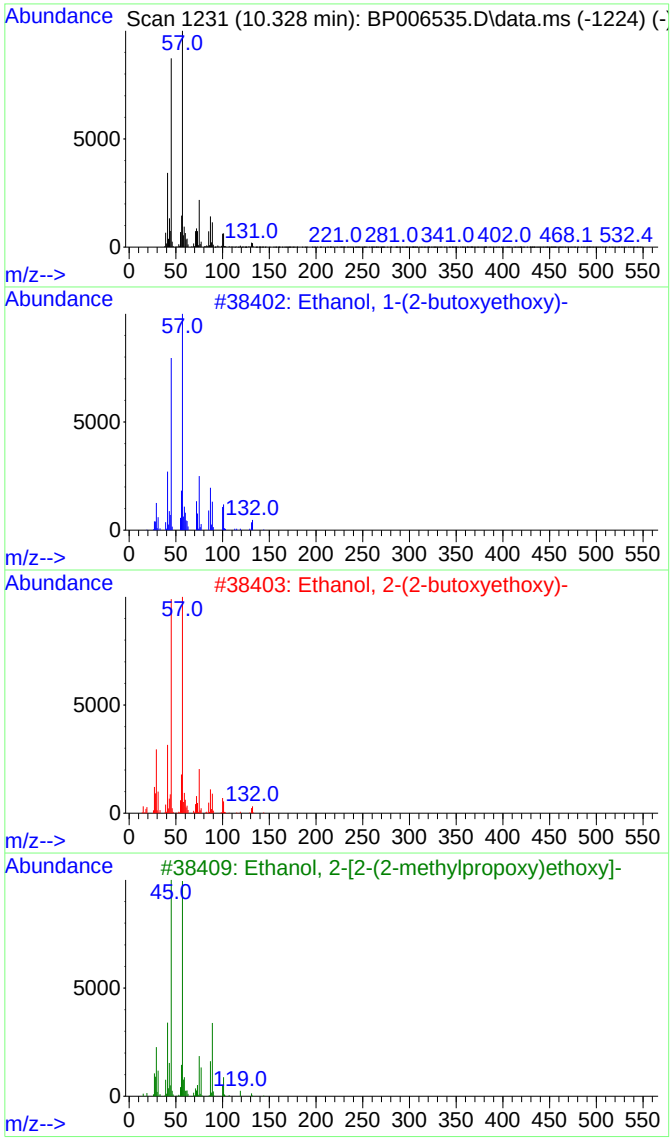
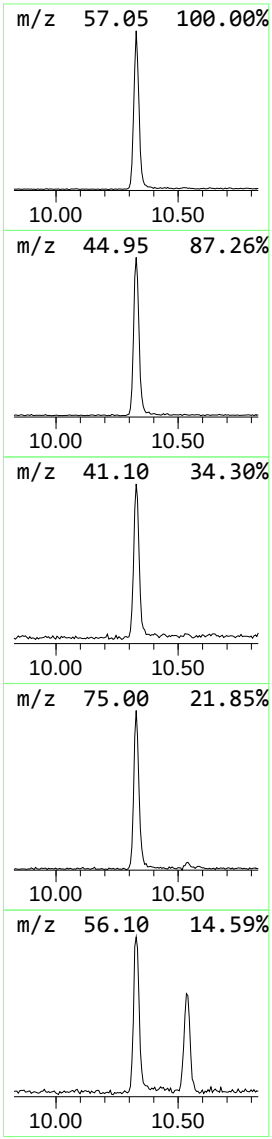
****
Peak Number 3 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	4.91 ng	440583	Naphthalene-d8	10.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
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-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50





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Misc :
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Instrument : BNA_P
ClientSampleId : TP-1

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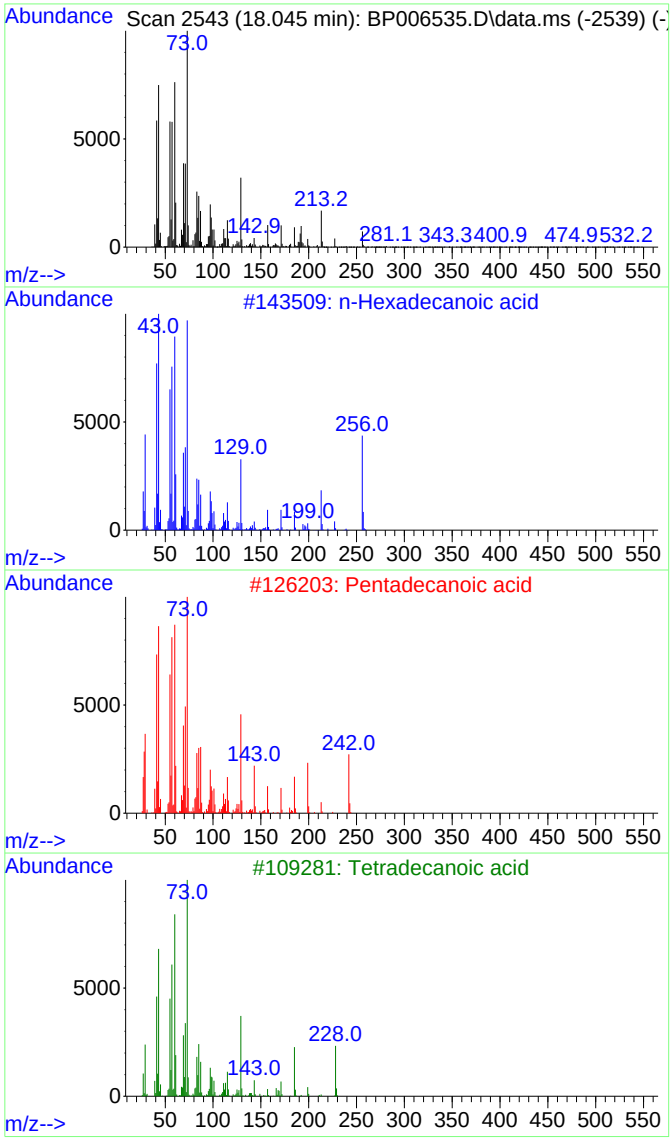
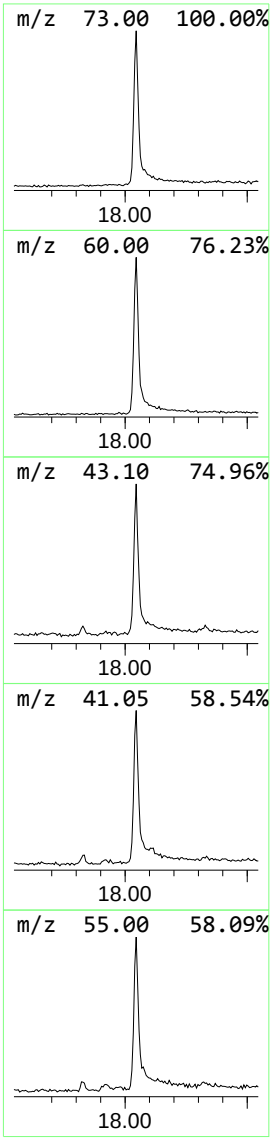
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	5.91 ng	749474	Phenanthrene-d10	17.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Isopropyl palmitate	298	C19H38O2	000142-91-6	64





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BNA_P
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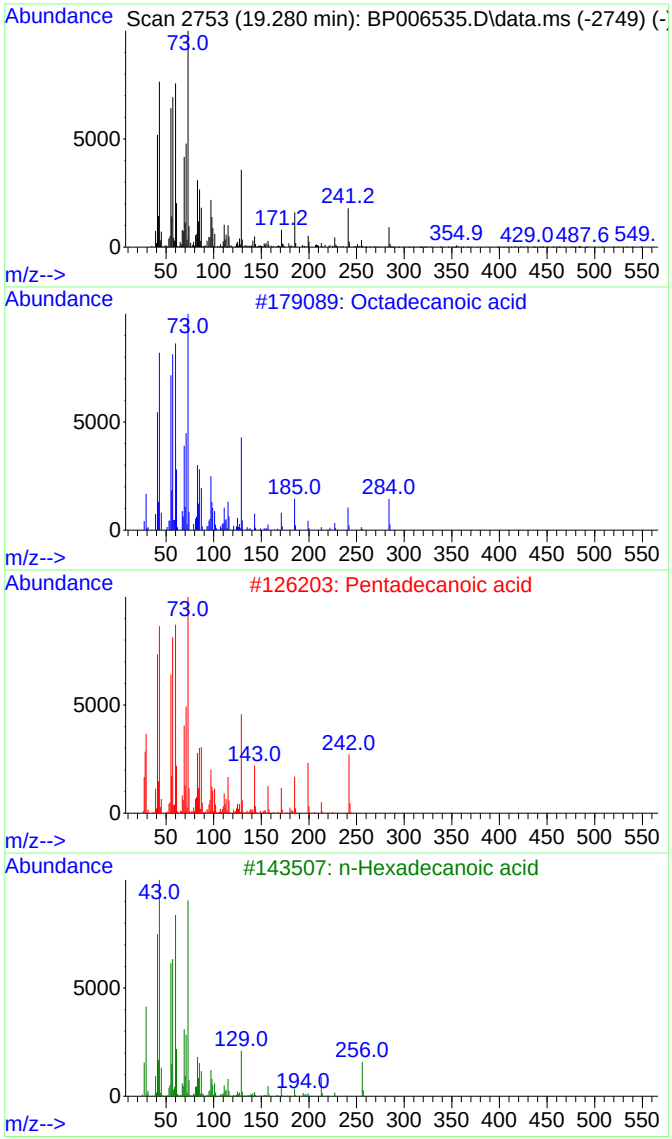
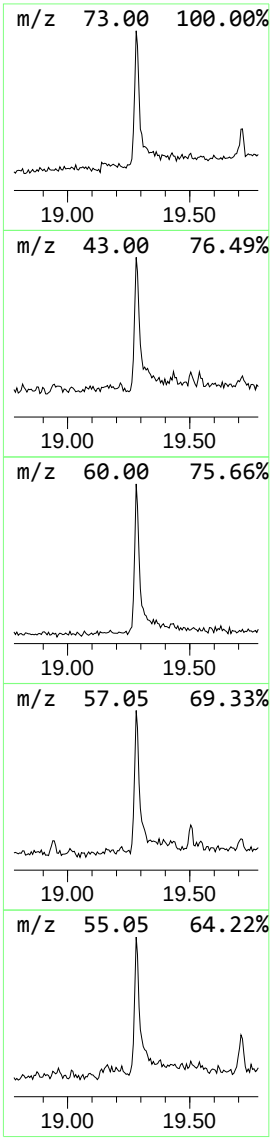
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.280	2.05 ng	329621	Chrysene-d12	21.233

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	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80





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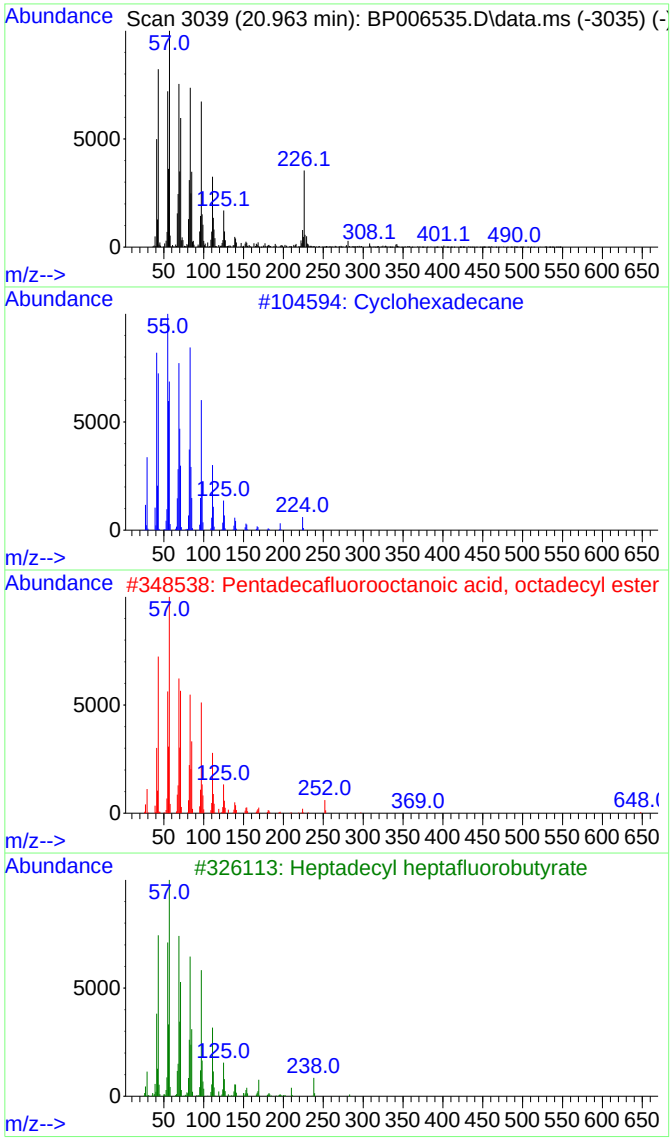
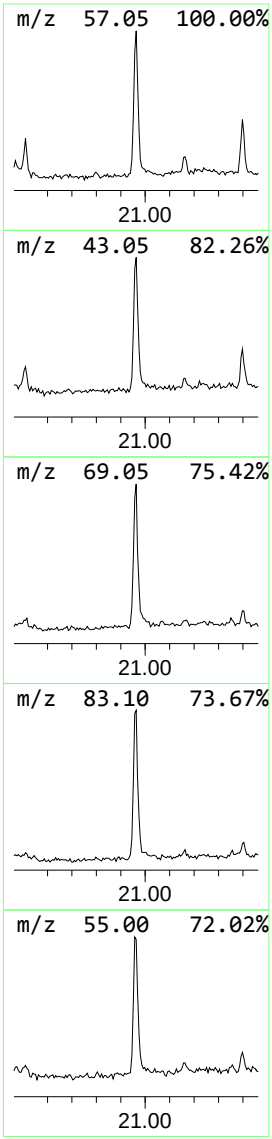
****

Peak Number 6 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.963	2.64 ng	424393	Chrysene-d12	21.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	94
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	93
5	1-Docosene	308	C22H44	001599-67-3	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
2-Pentanone, 4-...	4.905	22.7	ng	1452890	1	7.758	1279550	20.0
2-Pentanone, 4-...	5.969	4.7	ng	300124	1	7.758	1279550	20.0
Ethanol, 1-(2-b...	10.328	4.9	ng	440583	2	10.540	1792830	20.0
n-Hexadecanoic ...	18.045	5.9	ng	749474	4	17.134	2538290	20.0
Octadecanoic acid	19.280	2.0	ng	329621	5	21.233	3219330	20.0
Cyclohexadecane	20.963	2.6	ng	424393	5	21.233	3219330	20.0