LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061021\
Data File : BP005842.D
Acq On : 10 Jun 2021 17:35
Operator : CG/JU
Sample : M2637-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(246-248)

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-BP060821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005842.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.122	4	6	11	rVB	43353	47383	1.11%	0.225%
2	5.046	325	333	348	rBV	399890	565714	13.25%	2.684%
3	5.510	406	412	425	rBV	1252293	1879184	44.02%	8.915%
4	7.116	676	685	699	rBV	1218729	1944287	45.55%	9.223%
5	7.952	819	827	836	rBV	259746	412444	9.66%	1.957%
6	9.116	1017	1025	1038	rBV	731289	1244606	29.16%	5.904%
7	10.757	1296	1304	1321	rBV	292519	518848	12.15%	2.461%
8	13.204	1712	1720	1736	rBV	1878377	2822686	66.13%	13.390%
9	13.475	1759	1766	1773	rBV2	42869	70062	1.64%	0.332%
10	14.034	1854	1861	1872	rBV	260831	400139	9.37%	1.898%
11	14.575	1946	1953	1963	rBV	462617	673929	15.79%	3.197%
12	16.063	2199	2206	2228	rBV	1568367	2369592	55.51%	11.241%
13	17.322	2413	2420	2431	rBV	566824	828070	19.40%	3.928%
14	19.869	2847	2853	2858	rBV	3470005	4268616	100.00%	20.250%
15	20.533	2962	2966	2973	rVB	120170	142356	3.33%	0.675%
16	21.092	3057	3061	3070	rBV	310075	484497	11.35%	2.298%
17	21.392	3106	3112	3123	rBV	834246	1122935	26.31%	5.327%
18	23.810	3517	3523	3534	rVB2	651709	1284463	30.09%	6.093%

Sum of corrected areas: 21079811

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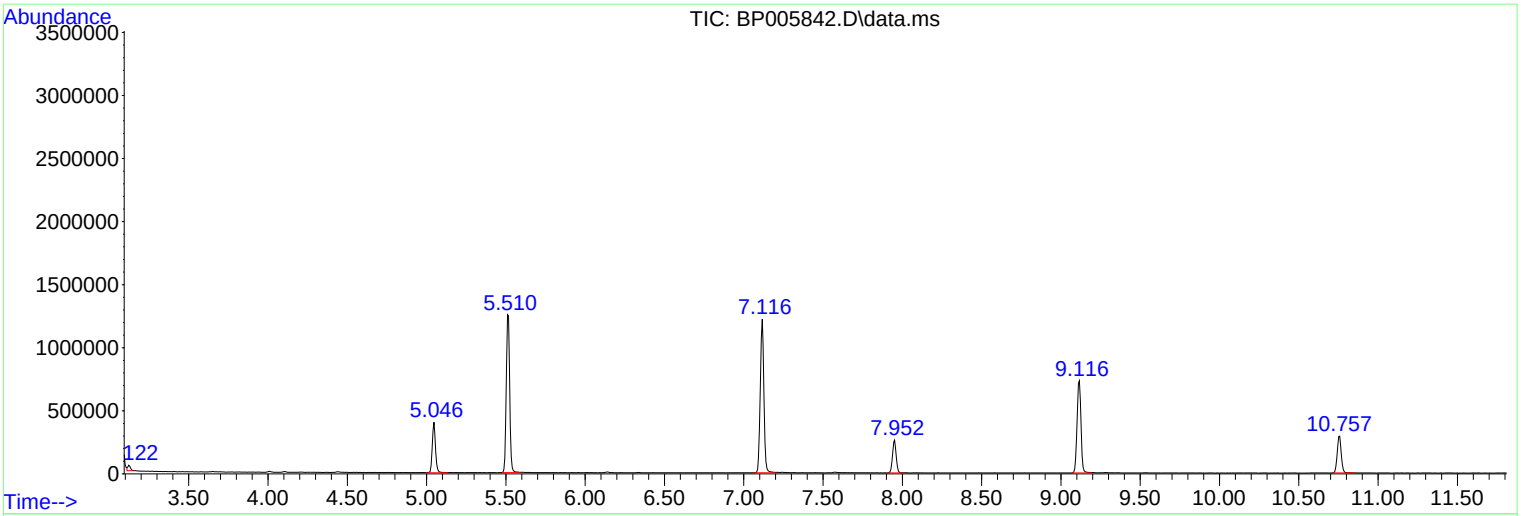
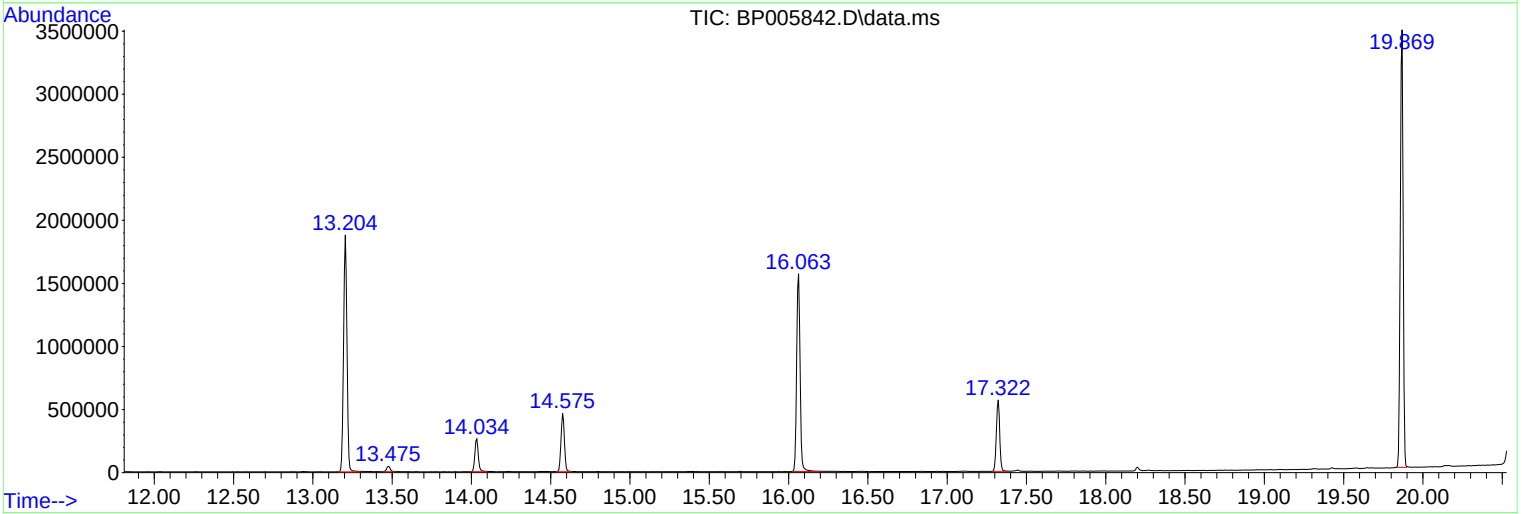
Misc :
ALS Vial : 14 Sample Multiplier: 1

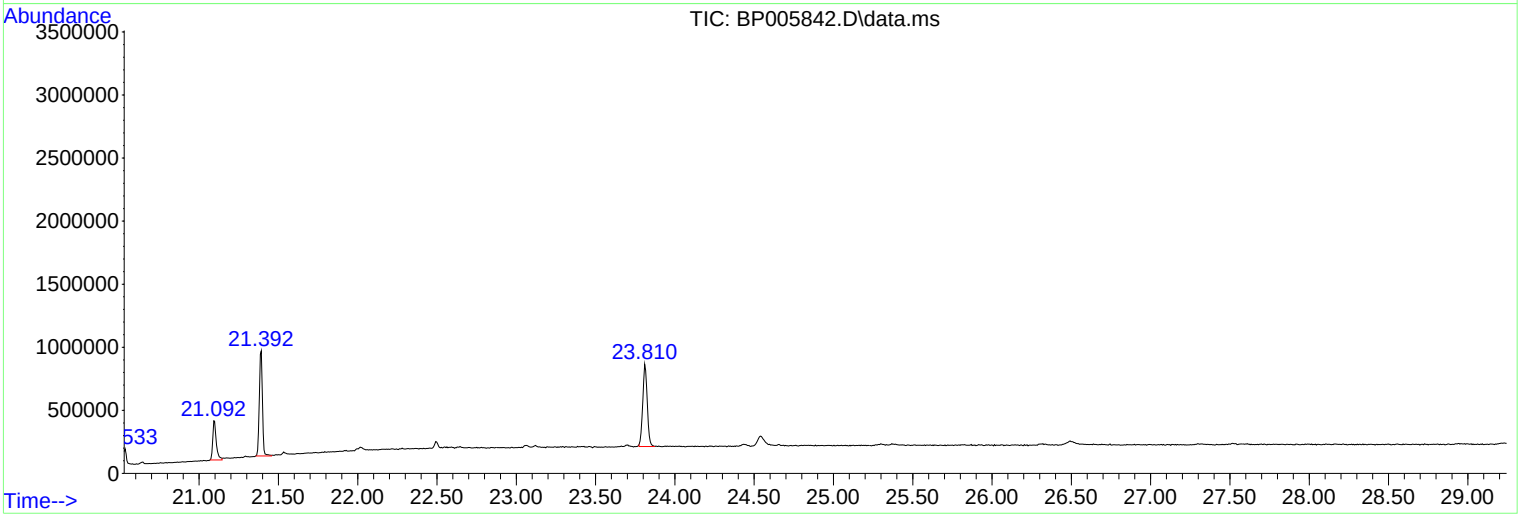
Instrument :
BNA_P
ClientSampleId :
18-B12(246-248)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Data File : BP005842.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

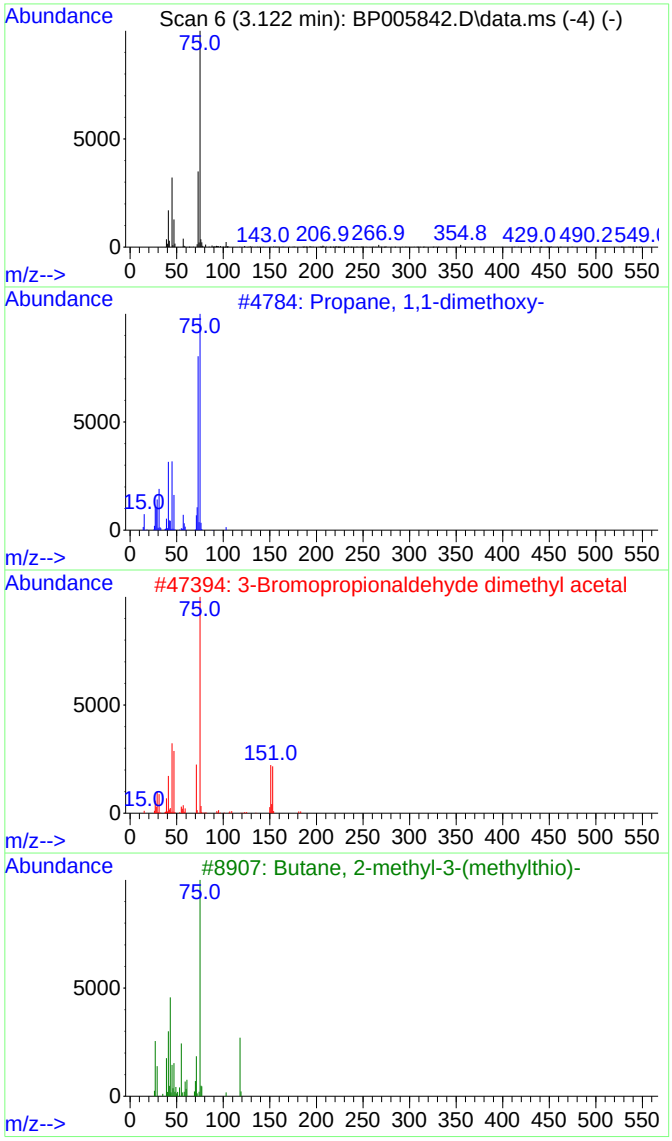
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

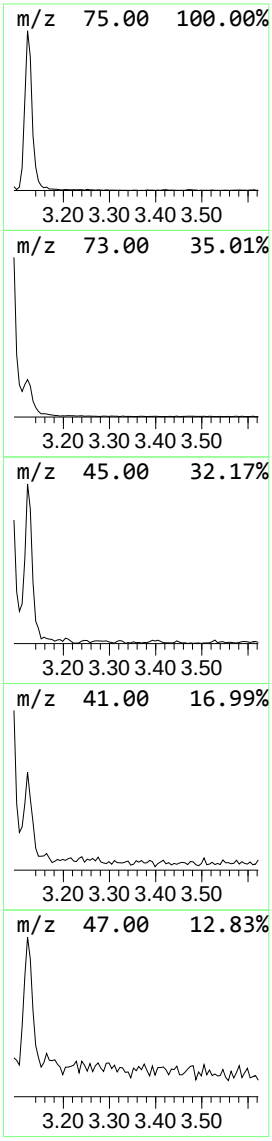
****

Peak Number 1 unknown3.122 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.122	2.30 ng	47383	1,4-Dichlorobenzene-d4	7.952

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	38
2	3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	36
3	Butane, 2-methyl-3-(methylthio)-	118	C6H14S	053897-51-1	36
4	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	36
5	Undecanal dimethyl acetal	216	C13H28O2	052517-67-6	9





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18-B12(246-248)

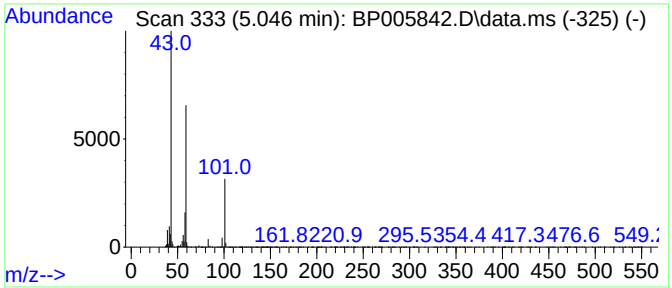
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

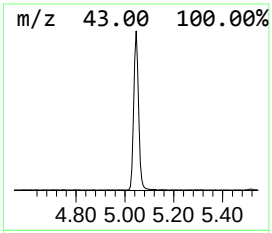
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

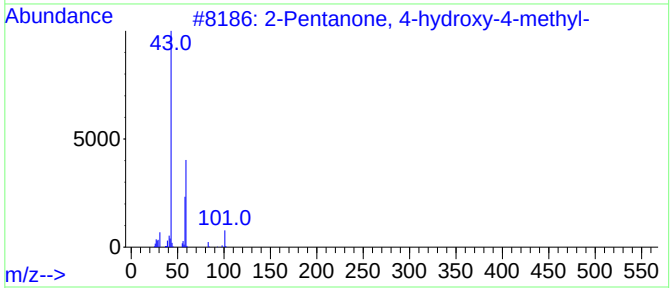
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

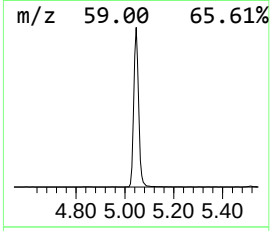
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	27.43 ng	565714	1,4-Dichlorobenzene-d4	7.952

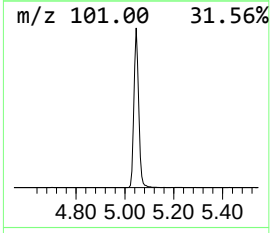
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9

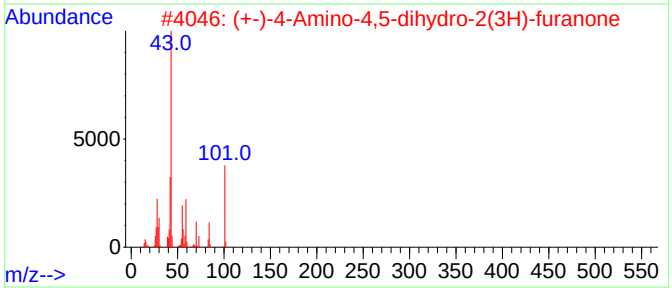


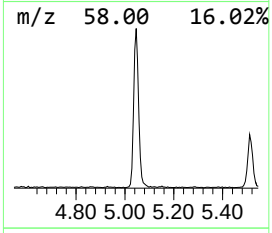


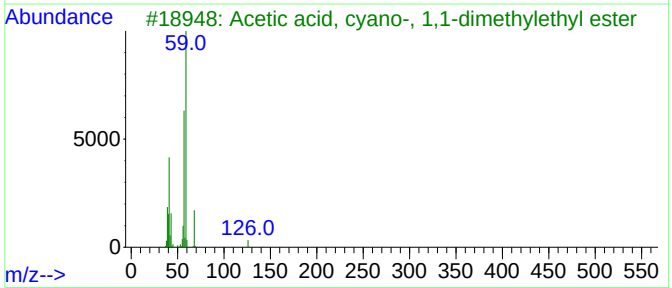


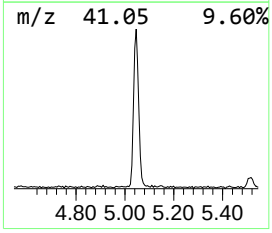












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ClientSampleId : 18-B12(246-248)

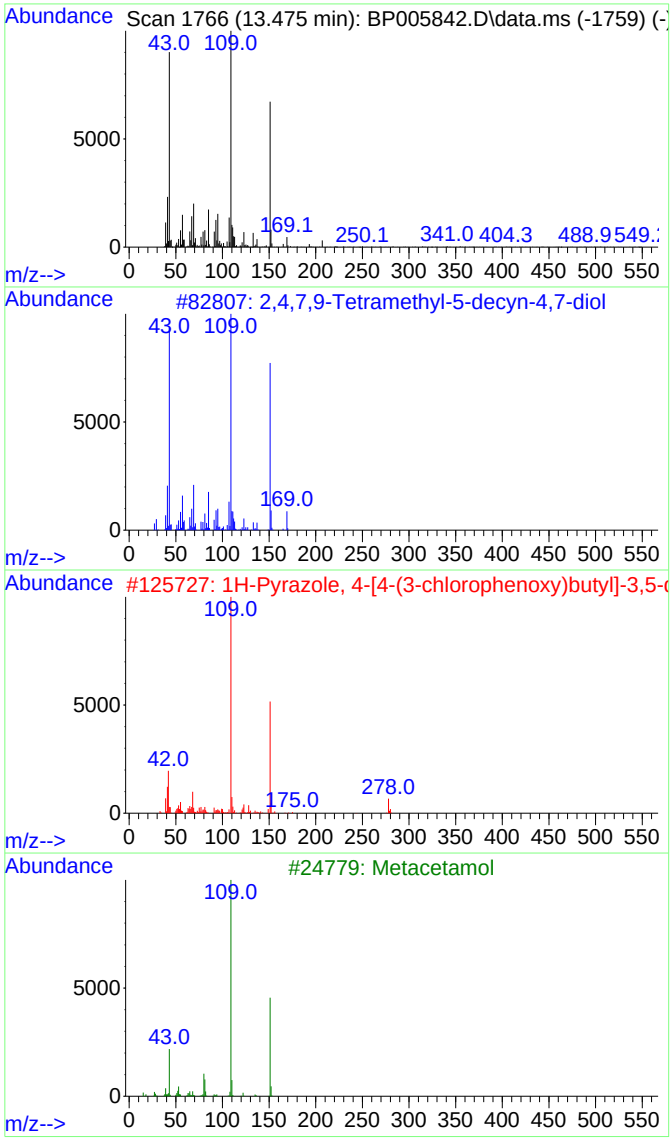
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

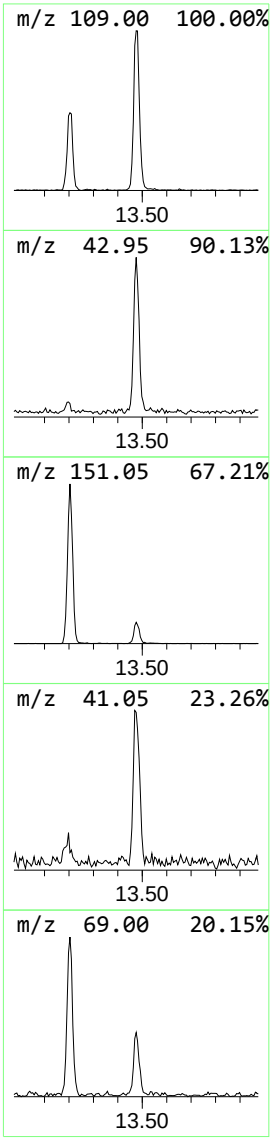
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.475	2.08 ng	70062	Acenaphthene-d10	14.575

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	1H-Pyrazole, 4-[4-(3-chloropheno...	278	C15H19ClN2O	1000302-33-9	59
3	Metacetamol	151	C8H9NO2	000621-42-1	53
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
5	Cyclohexanemethanol, 3,3-dimethy...	212	C13H24O2	072541-28-7	52





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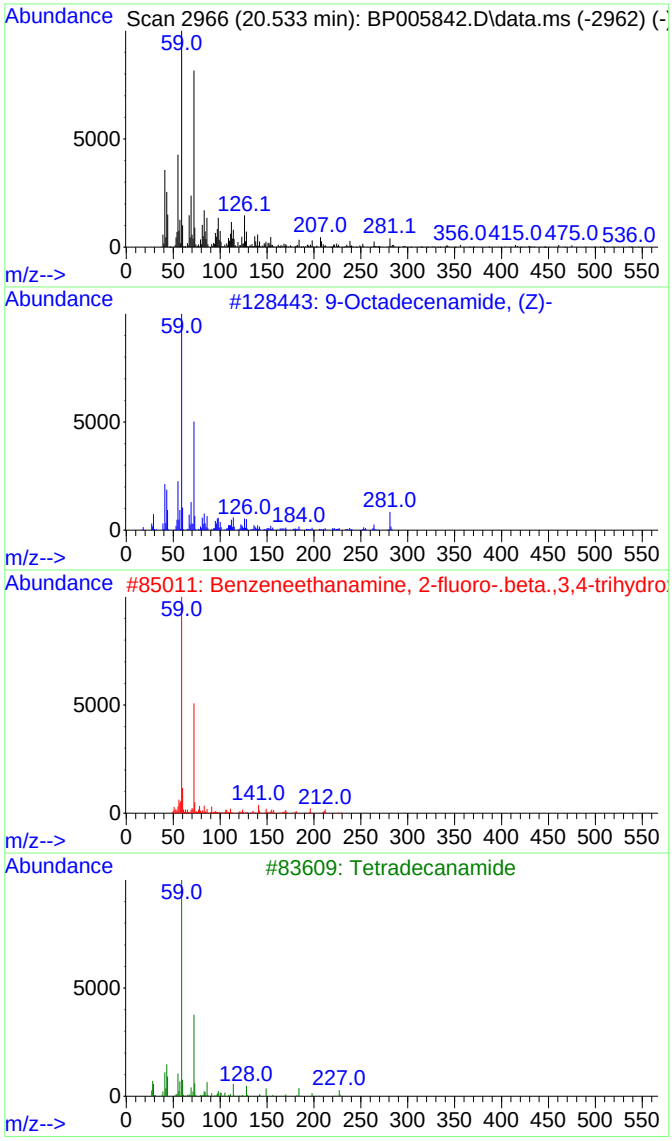
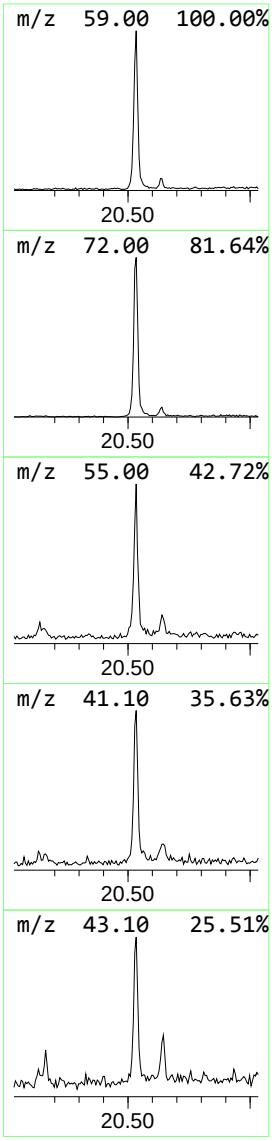
****

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.533	2.54 ng	142356	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	43
3	Tetradecanamide	227	C14H29NO	000638-58-4	38
4	Nonanamide	157	C9H19NO	001120-07-6	38
5	Octanamide	143	C8H17NO	000629-01-6	38





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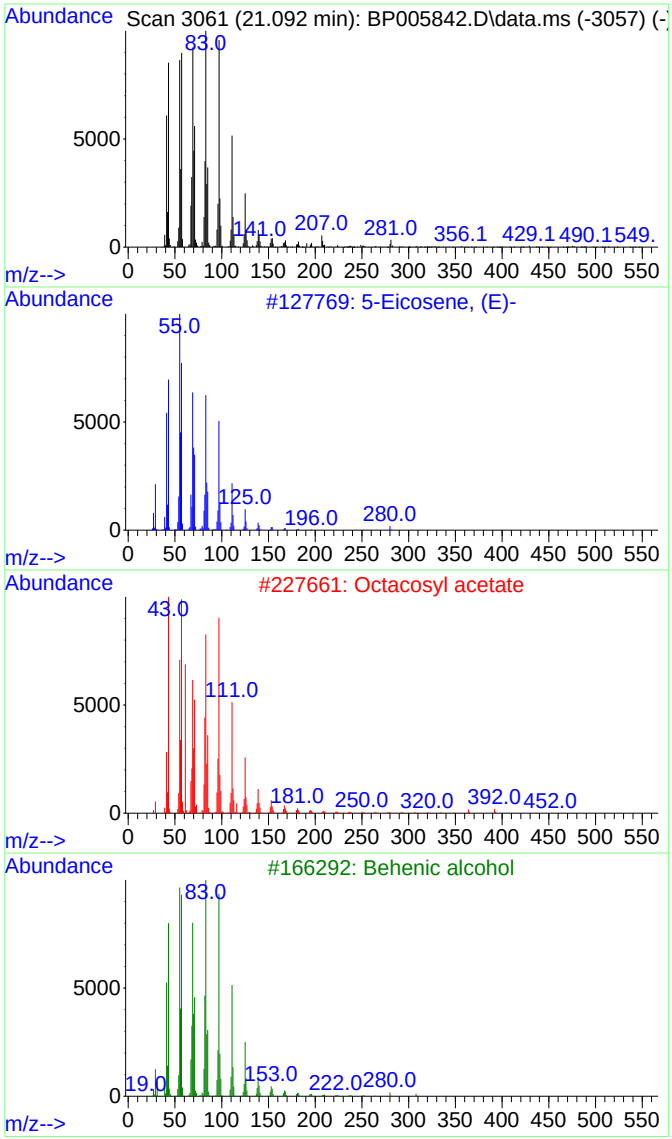
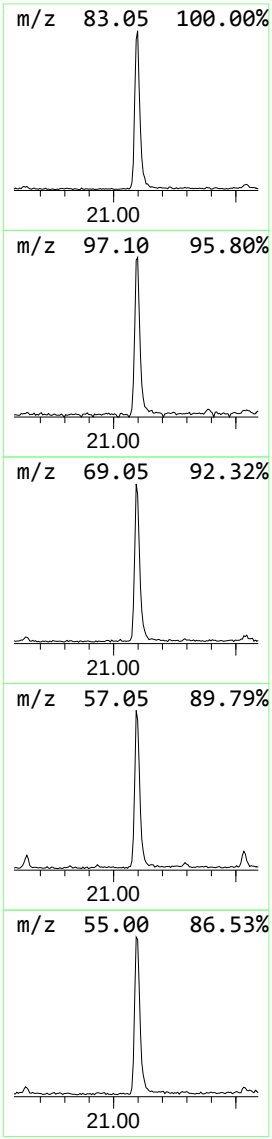
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	8.63 ng	484497	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	Octacosyl acetate	452	C30H60O2	018206-97-8	97
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94





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
unknown3.122	3.122	2.3	ng	47383	1	7.952	412444	20.0
2-Pentanone, 4-...	5.046	27.4	ng	565714	1	7.952	412444	20.0
2,4,7,9-Tetrame...	13.475	2.1	ng	70062	3	14.575	673929	20.0
9-Octadecenamid...	20.533	2.5	ng	142356	5	21.392	1122940	20.0
5-Eicosene, (E)-	21.092	8.6	ng	484497	5	21.392	1122940	20.0