LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111622\
Data File : BF131269.D
Acq On : 16 Nov 2022 17:18
Operator : CG\JU
Sample : N5497-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-11

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_F\Methods\8270-BF111522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.281	26	33	38	rVB	1682921	2159235	75.62%	11.769%
2	2.387	47	51	60	rVB	35957	48542	1.70%	0.265%
3	4.081	335	339	344	rVB	53255	66053	2.31%	0.360%
4	4.581	419	424	428	rVB	106439	113302	3.97%	0.618%
5	5.187	522	527	533	rVB	265717	278802	9.76%	1.520%
6	5.575	588	593	596	rBV	1397683	1219659	42.71%	6.648%
7	6.575	759	763	766	rBV	889202	762036	26.69%	4.153%
8	6.969	827	830	834	rBV	582162	501799	17.57%	2.735%
9	7.540	921	927	930	rBV	1687975	1665831	58.34%	9.080%
10	8.263	1045	1050	1053	rBV	735116	639643	22.40%	3.486%
11	9.345	1228	1234	1237	rBV	3245192	2855400	100.00%	15.563%
12	10.028	1346	1350	1353	rBV	891783	697475	24.43%	3.802%
13	10.822	1480	1485	1488	rBV	1816743	1607095	56.28%	8.759%
14	11.157	1531	1542	1543	rBV3	37273	94134	3.30%	0.513%
15	11.522	1601	1604	1608	rBV	776195	680549	23.83%	3.709%
16	12.045	1689	1693	1697	rBV	85710	80343	2.81%	0.438%
17	12.751	1809	1813	1814	rBV	304887	348343	12.20%	1.899%
18	12.769	1814	1816	1825	rVV	796533	855051	29.95%	4.660%
19	12.839	1825	1828	1839	rVB2	118477	146989	5.15%	0.801%
20	13.122	1872	1876	1879	rBV	1822849	1527942	53.51%	8.328%
21	13.457	1927	1933	1935	rBV	151350	150330	5.26%	0.819%
22	14.092	2035	2041	2048	rBV5	33441	100286	3.51%	0.547%
23	14.180	2052	2056	2061	rVB	432086	374580	13.12%	2.042%
24	14.280	2067	2073	2082	rVB5	28691	61343	2.15%	0.334%
25	14.757	2146	2154	2165	rBV6	85136	409201	14.33%	2.230%
26	15.663	2300	2308	2313	rBV6	81048	271508	9.51%	1.480%
27	15.727	2314	2319	2334	rVB	385574	589881	20.66%	3.215%
28	17.068	2538	2547	2548	rBV7	18690	41793	1.46%	0.228%

Sum of corrected areas: 18347145

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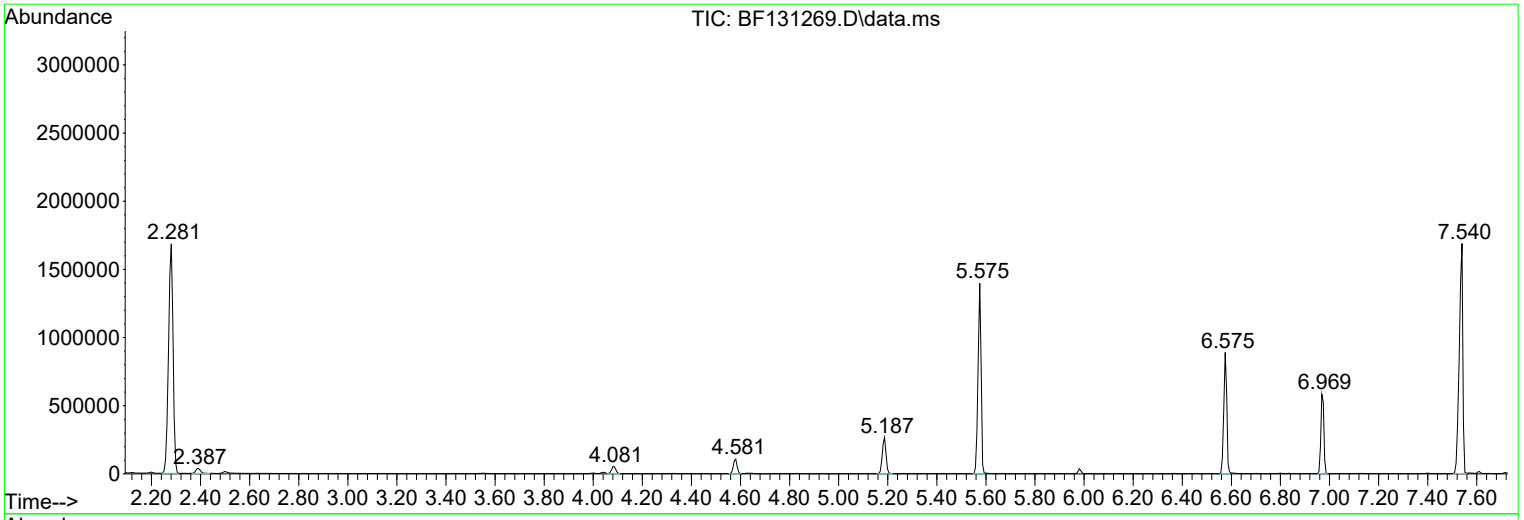
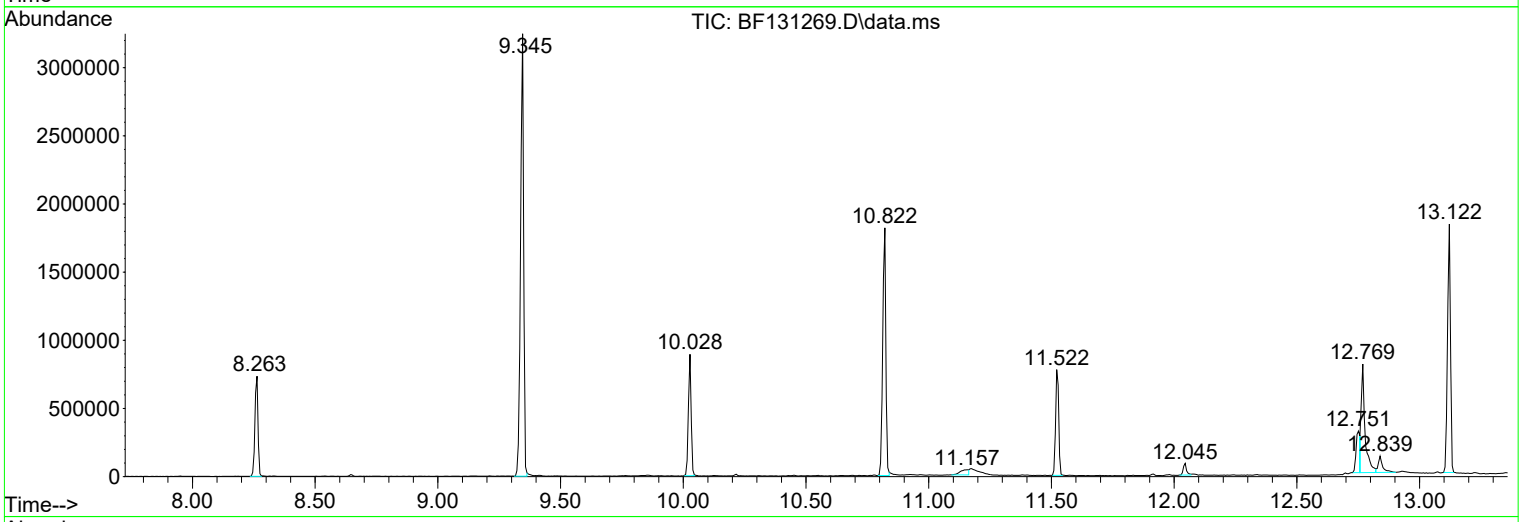
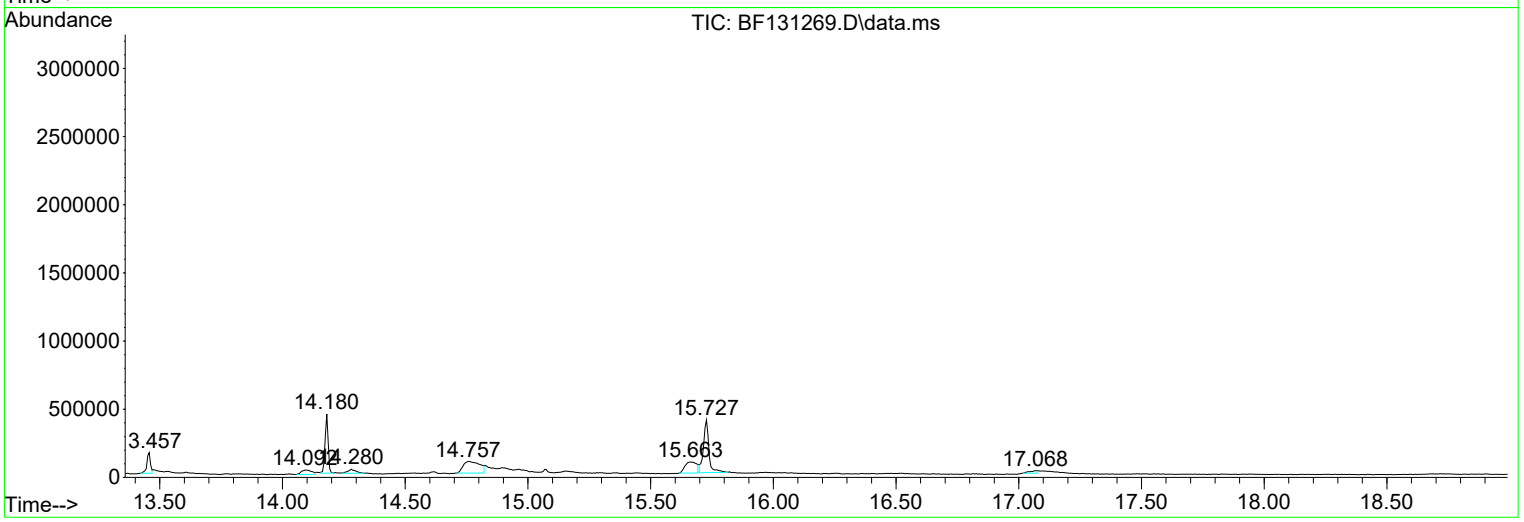
ClientSampleId :
MW-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.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

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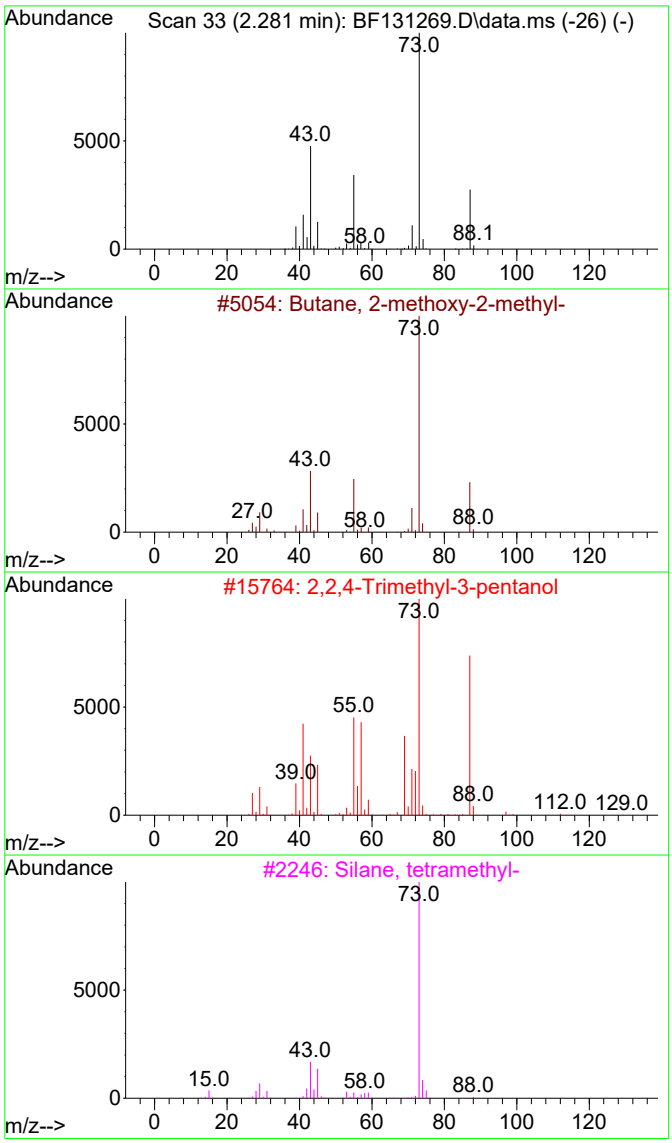
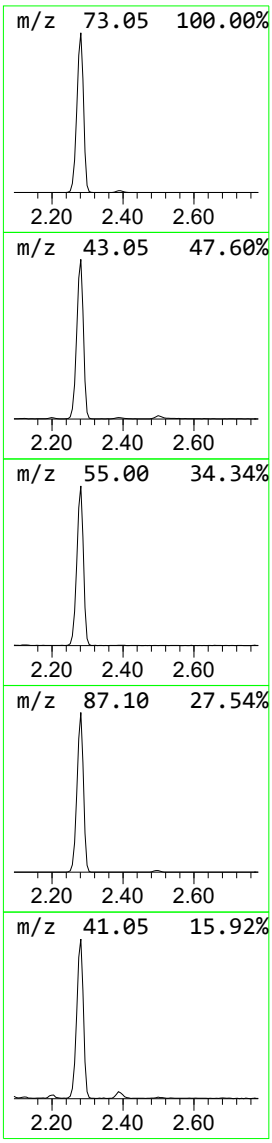
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	86.06 ng	2159240	1,4-Dichlorobenzene-d4	6.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.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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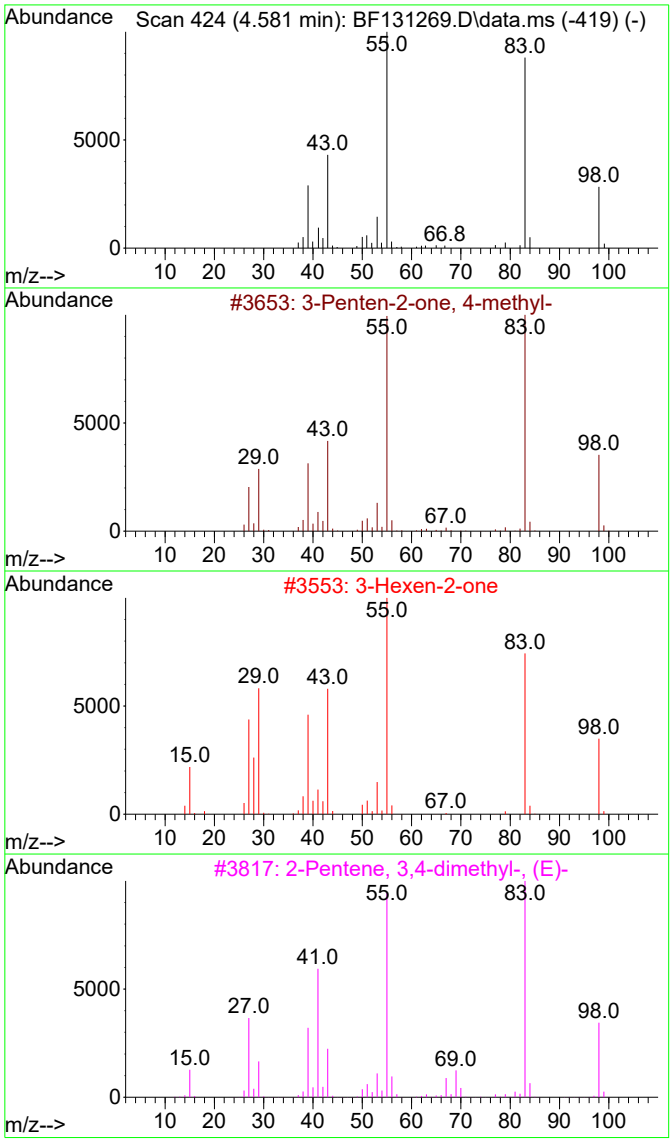
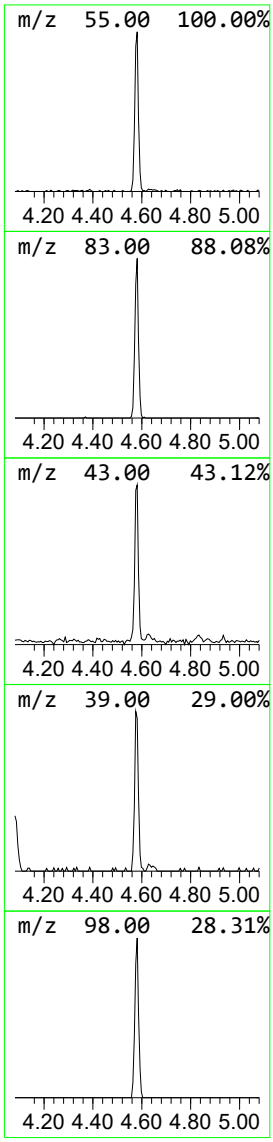
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.581	4.52 ng	113302	1,4-Dichlorobenzene-d4	6.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86





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Operator : CG\JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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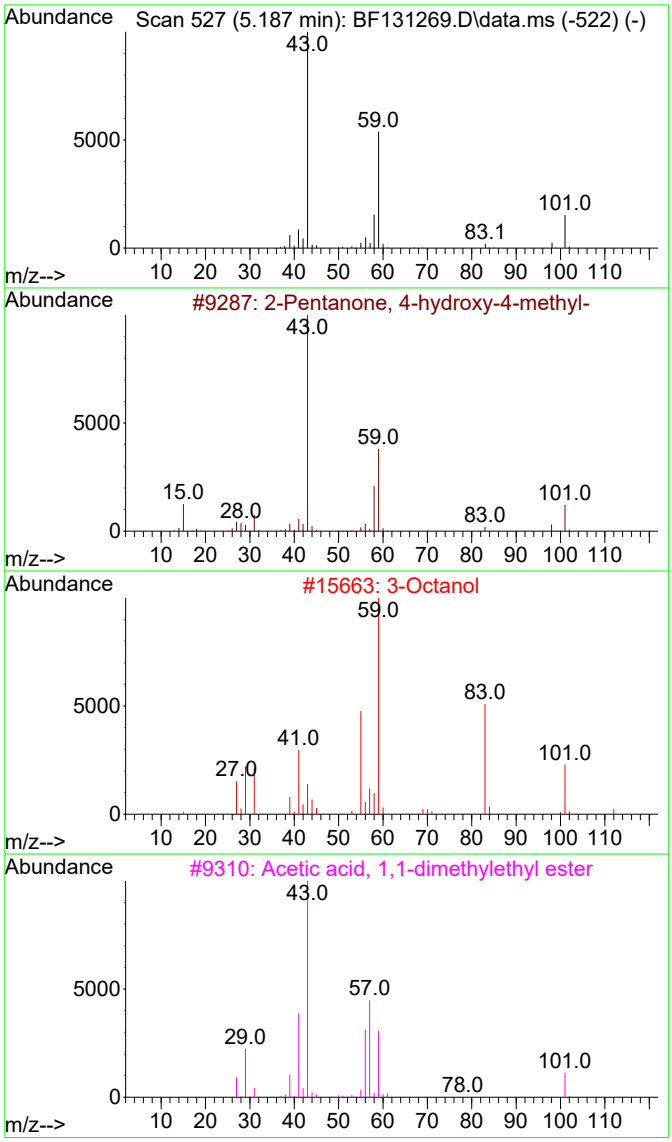
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

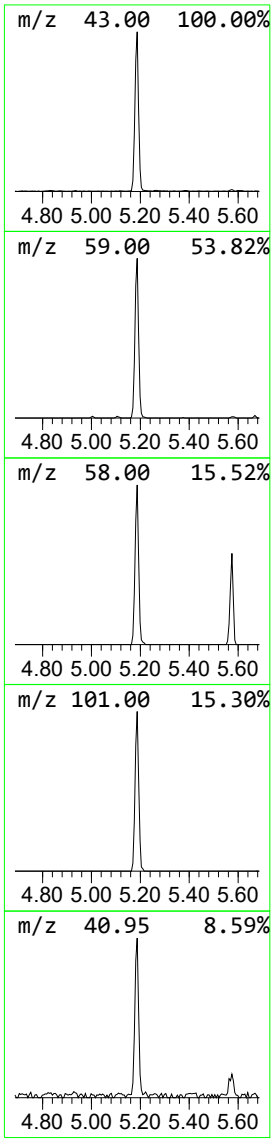
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	11.11 ng	278802	1,4-Dichlorobenzene-d4	6.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Octanol	130	C8H18O	000589-98-0	36
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.M
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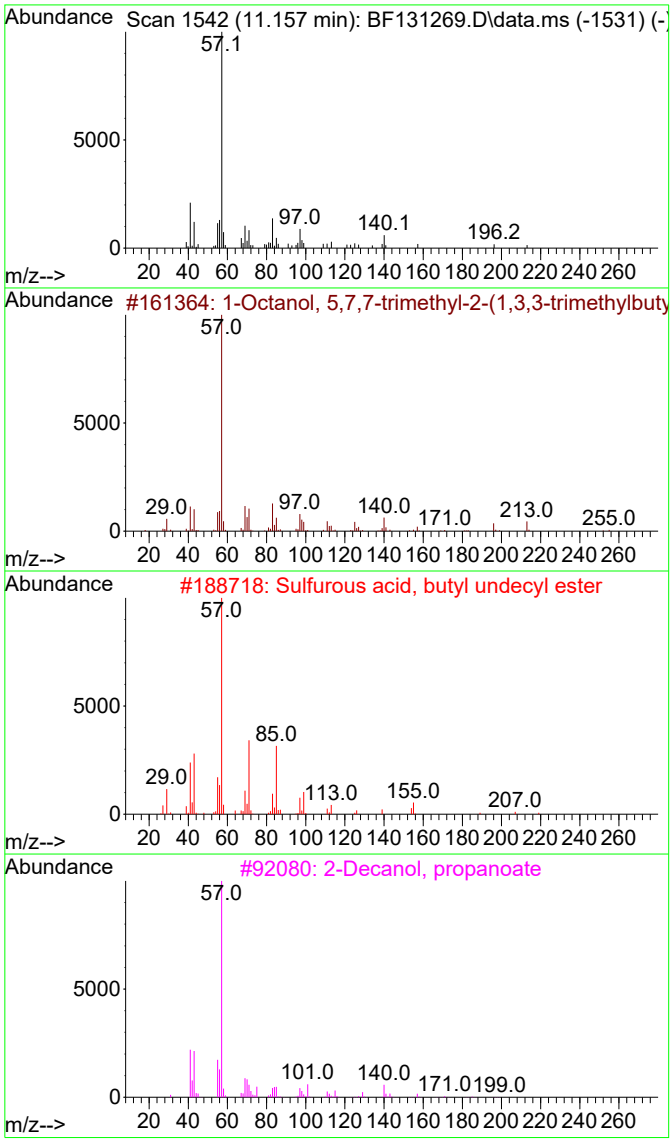
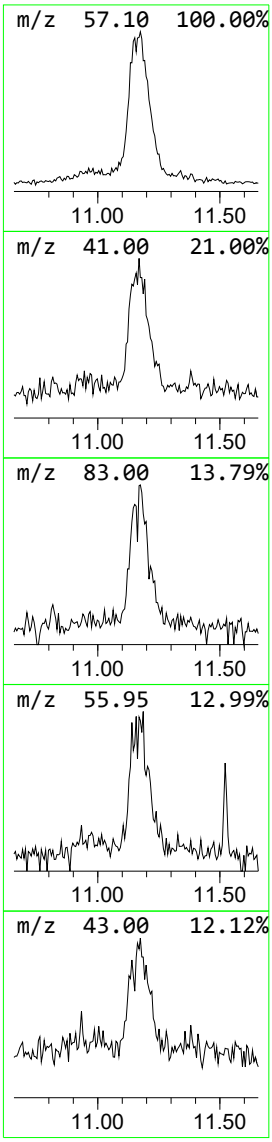
****
Peak Number 5 1-Octanol, 5,7,7-trimethyl-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.157	2.77 ng	94134	Phenanthrene-d10	11.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	59
2	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	59
3	2-Decanol, propanoate	214	C13H26O2	055683-11-9	53
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	53
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	53





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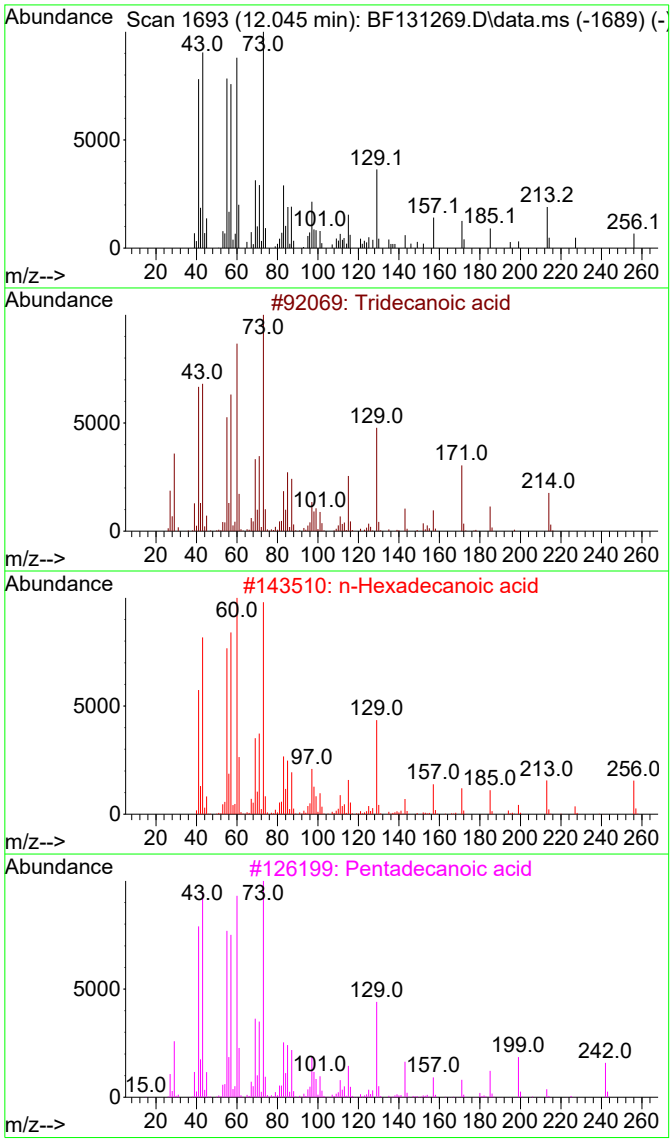
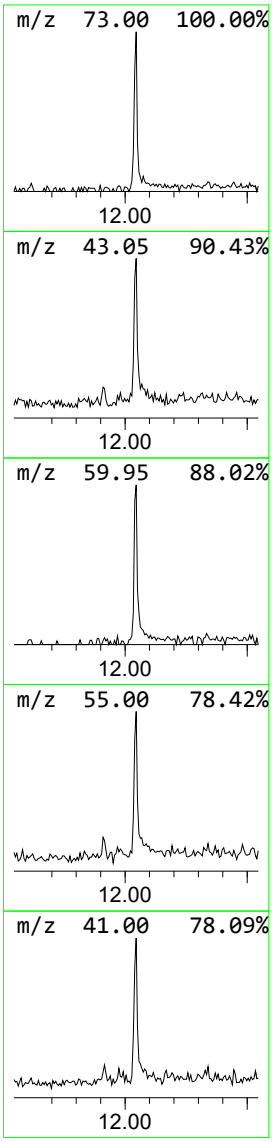
****

Peak Number 6 Tridecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.045	2.36 ng	80343	Phenanthrene-d10	11.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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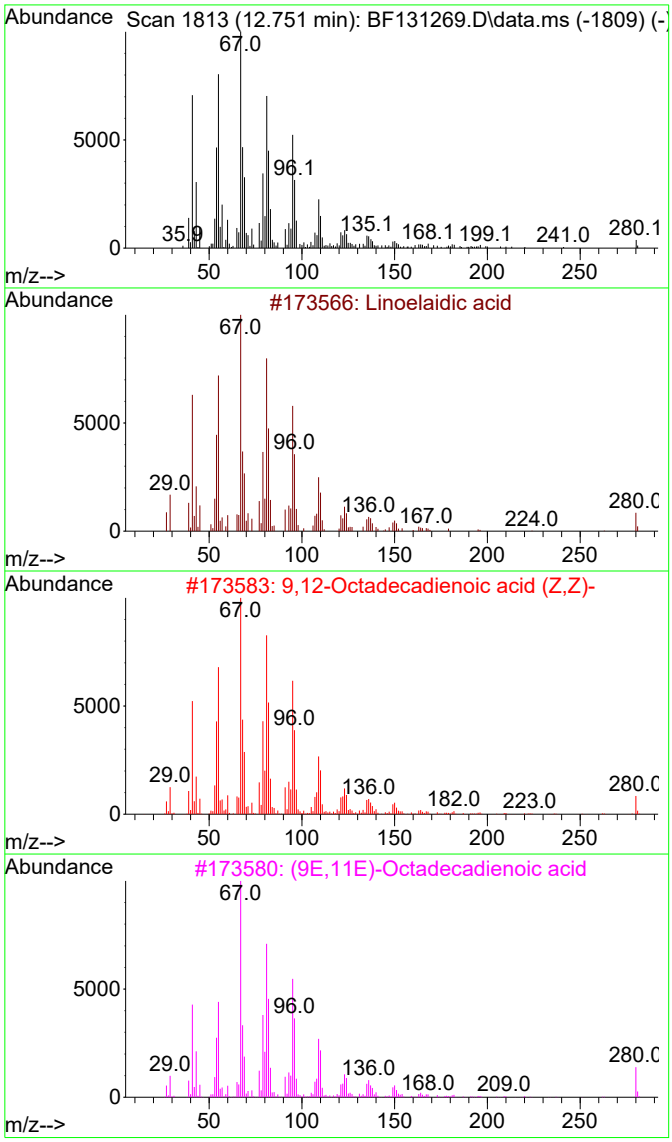
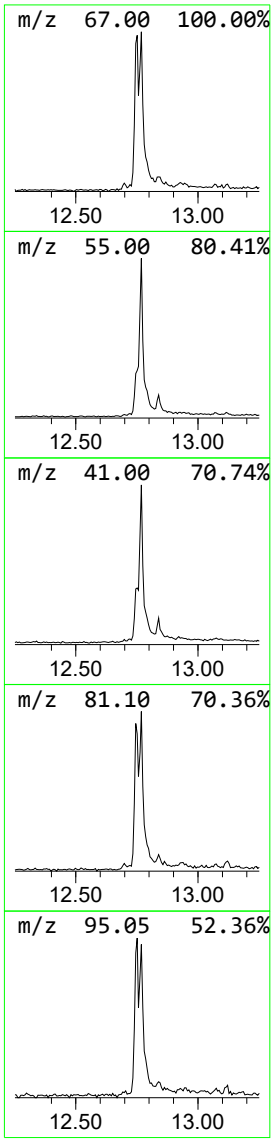
****

Peak Number 7 Linoelaidic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	10.24 ng	348343	Phenanthrene-d10	11.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Linoelaidic acid	280	C18H32O2	000506-21-8	99
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
3	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	98
4	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	97
5	11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	91





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Sample : N5497-04
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ClientSampleId :
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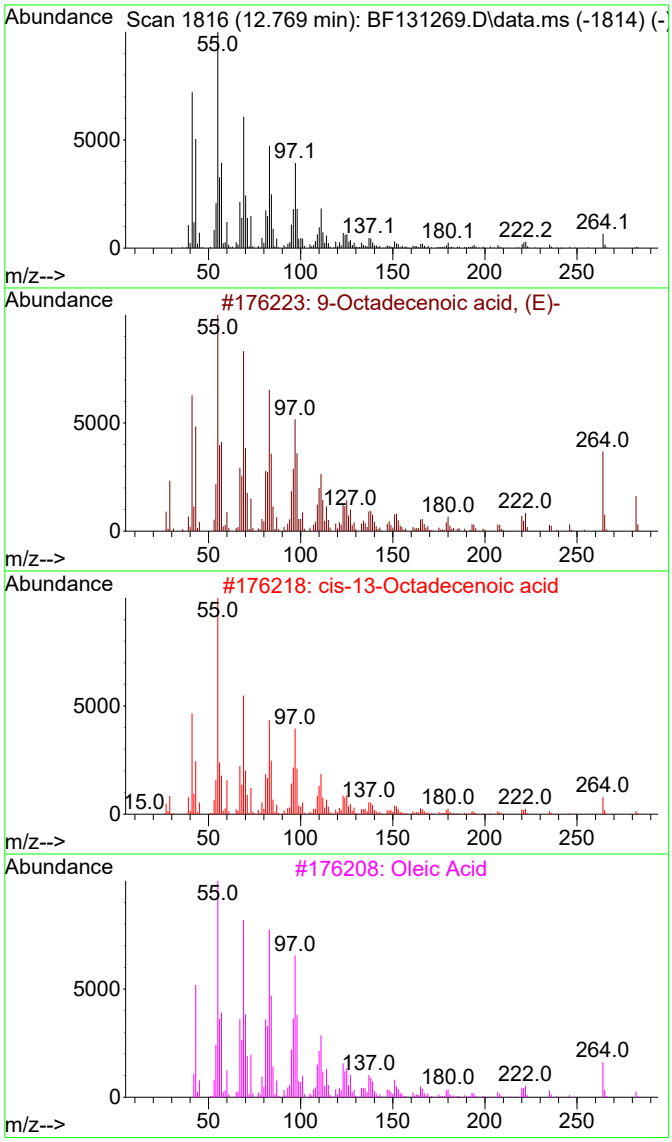
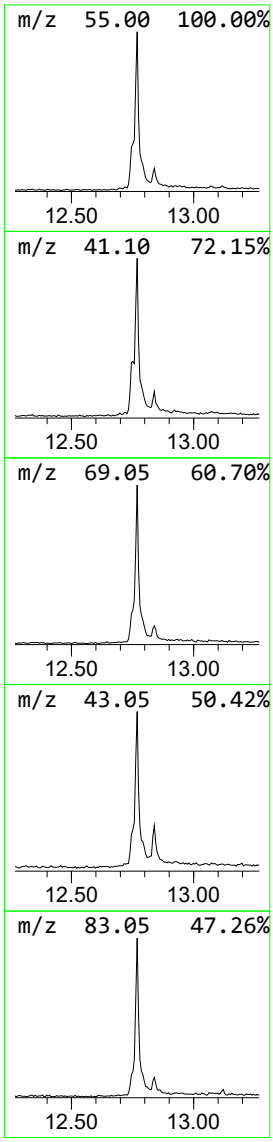
Peak Number 8 9-Octadecenoic acid, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.769	25.13 ng	855051	Phenanthrene-d10	11.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	95
2	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91
3	Oleic Acid	282	C18H34O2	000112-80-1	91
4	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	87
5	Palmitoleic acid	254	C16H30O2	000373-49-9	87





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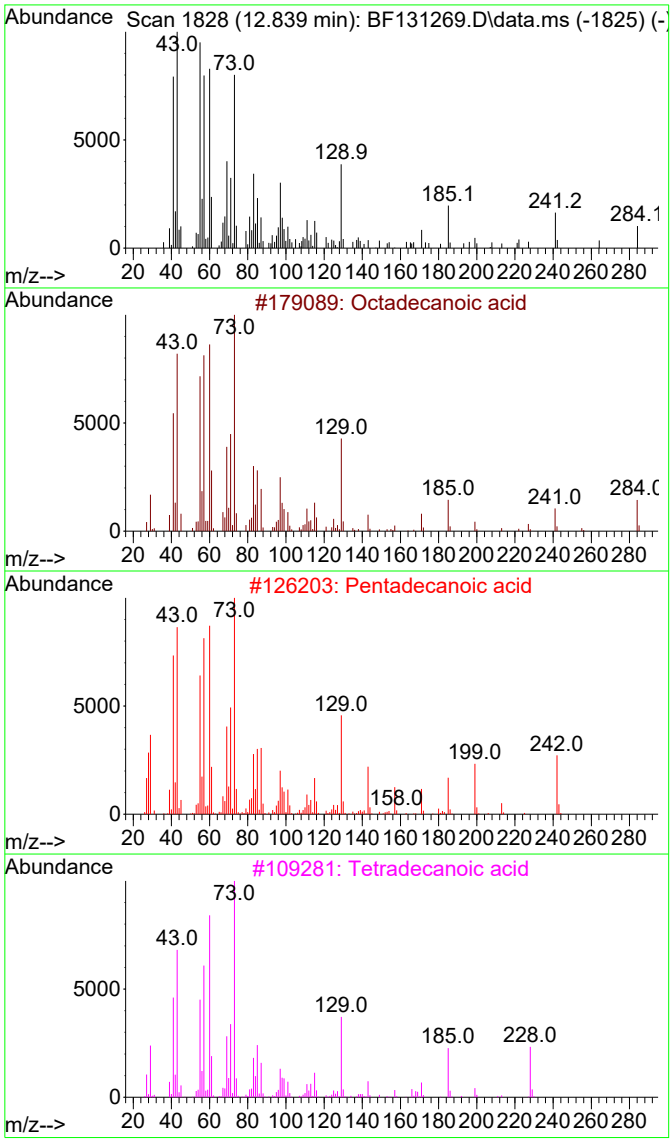
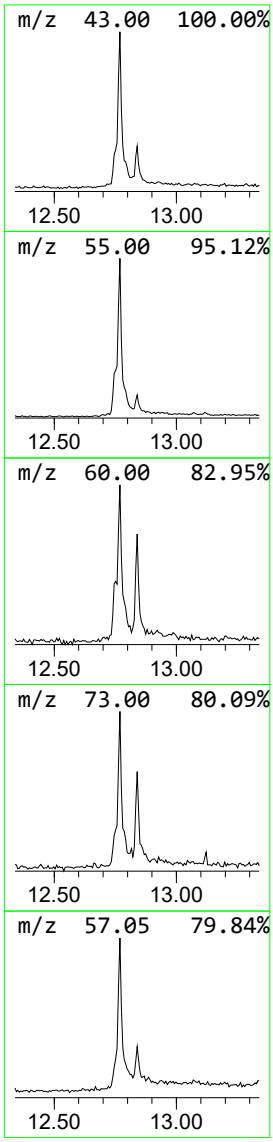
Peak Number 9 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.839	4.32 ng	146989	Phenanthrene-d10	11.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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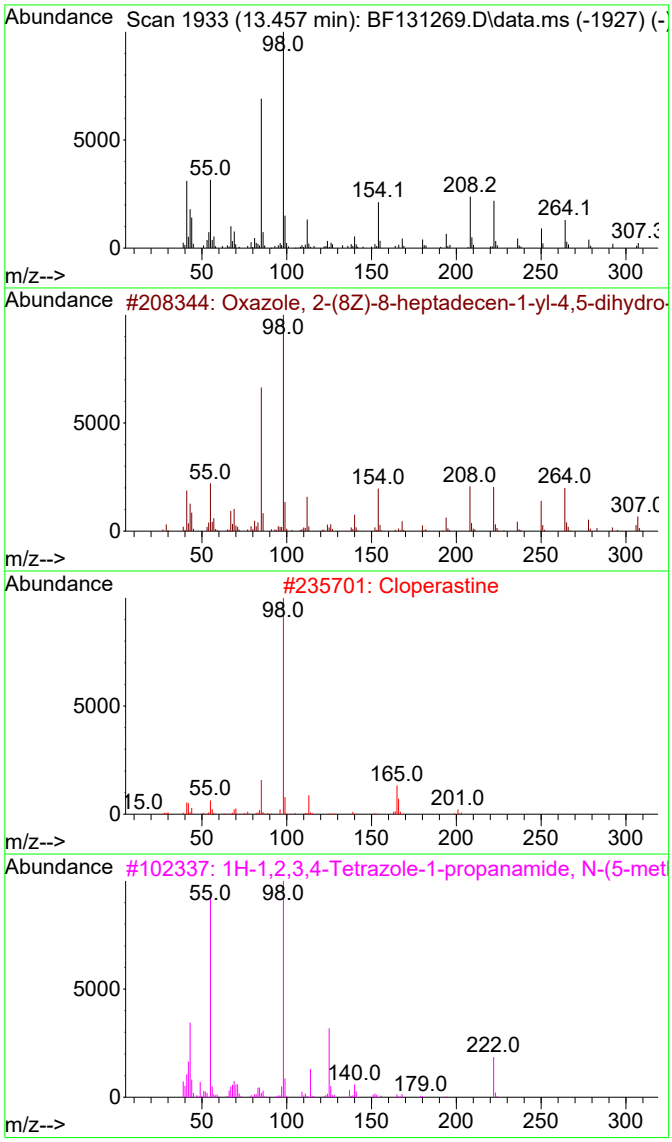
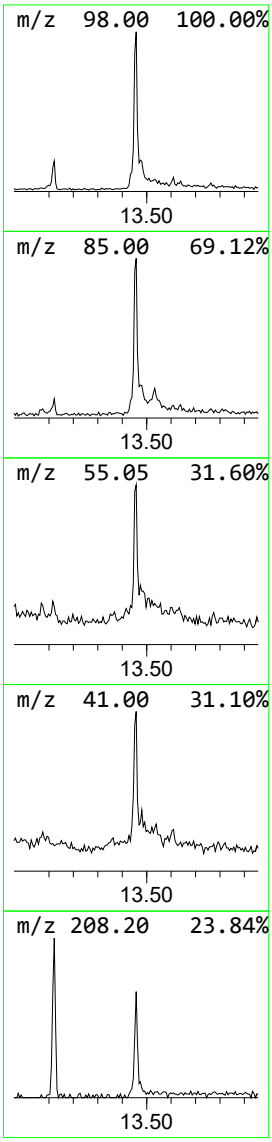
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Oxazole, 2-(8Z)-8-heptadece... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	8.03 ng	150330	Chrysene-d12	14.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazole, 2-(8Z)-8-heptadecen-1-y...	307	C20H37NO	034900-26-0	99
2	Cloperastine	329	C20H24ClNO	003703-76-2	35
3	1H-1,2,3,4-Tetrazole-1-propanami...	222	C8H10N6O2	1000349-93-9	35
4	1,2-Dihydro-3-methoxy-2-oxo-1-pi...	222	C12H18N2O2	020928-62-5	35
5	Isoindole-1,3,5-trione, perhydro...	278	C15H22N2O3	1000266-79-5	27





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Data File : BF131269.D
Acq On : 16 Nov 2022 17:18
Operator : CG\JU
Sample : N5497-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.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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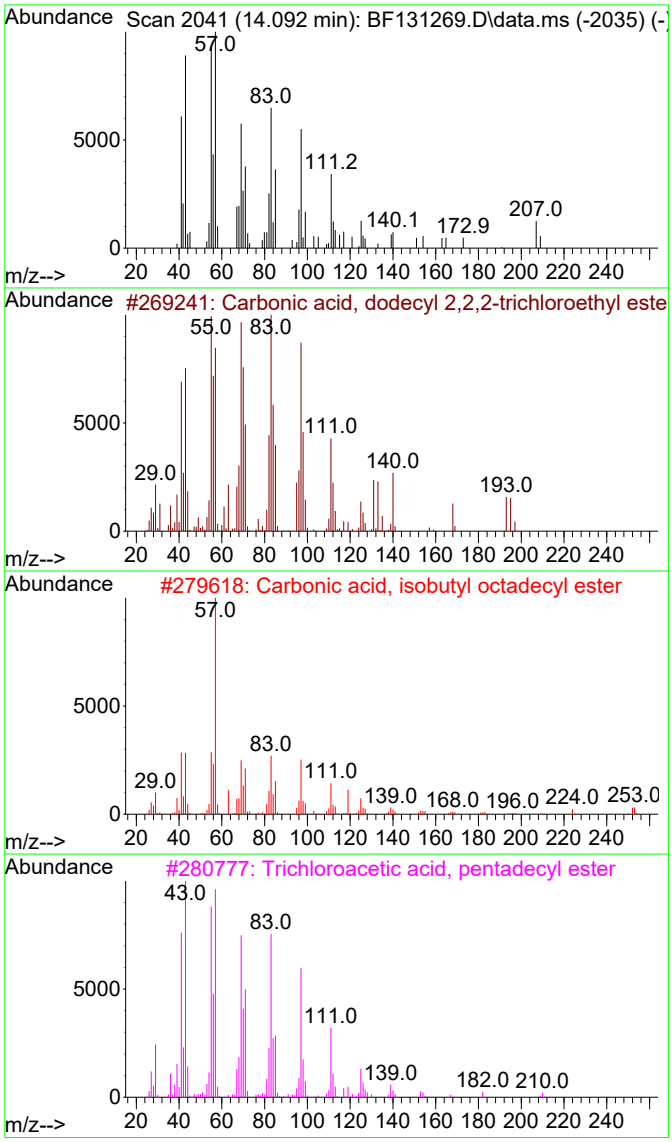
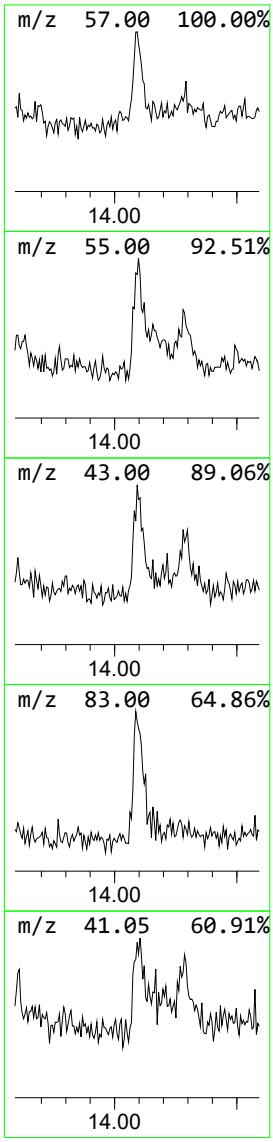
Peak Number 11 Carbonic acid, dodecyl 2,2,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	5.35 ng	100286	Chrysene-d12	14.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, dodecyl 2,2,2-tri...	360	C15H27Cl3O3	1000314-55-8	91
2	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	90
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	80
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	80





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Data File : BF131269.D
Acq On : 16 Nov 2022 17:18
Operator : CG\JU
Sample : N5497-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.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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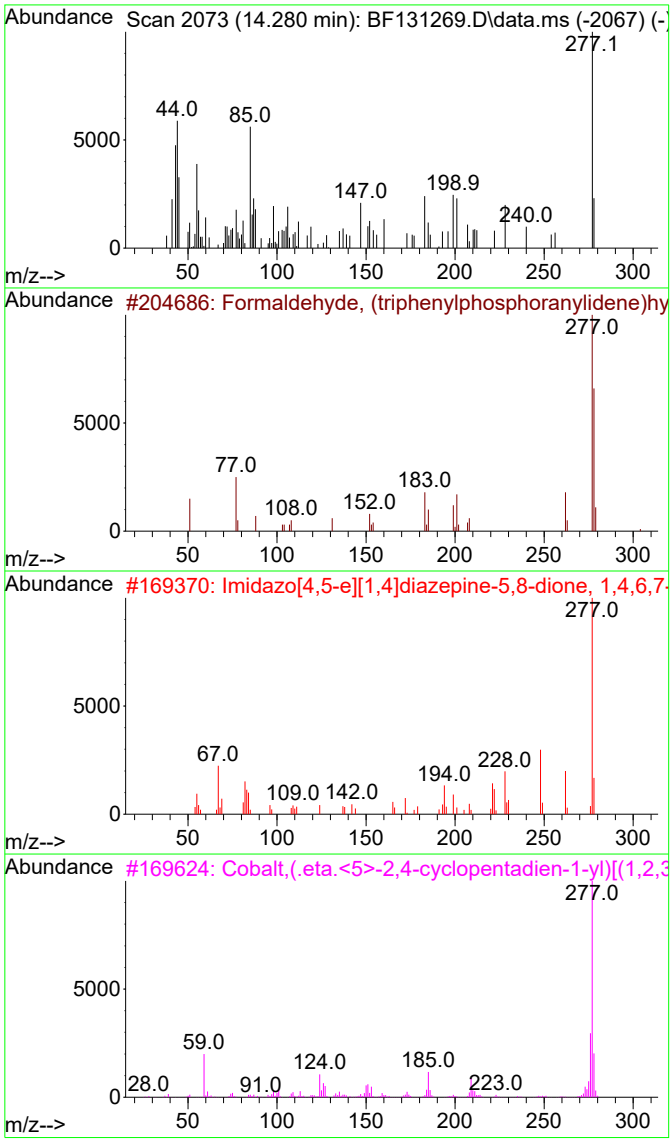
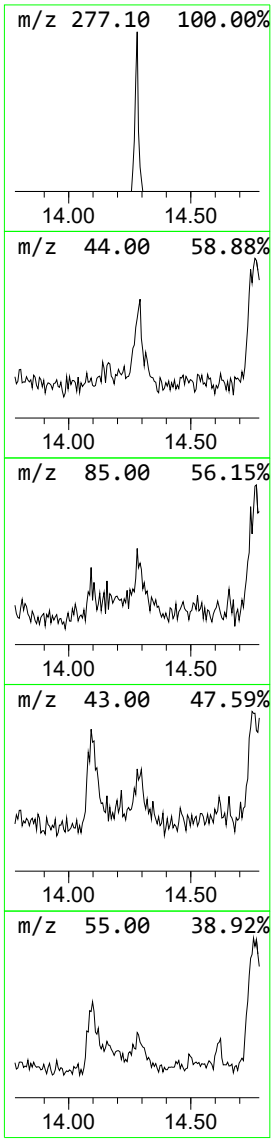
Peak Number 12 unknown14.280 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.280	3.28 ng	61343	Chrysene-d12	14.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	25
2	Imidazo[4,5-e][1,4]diazepine-5,8...	277	C13H19N5O2	1000142-45-4	25
3	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	25
4	2-(1,3-Benzodiazol-1-yl)-5-(trif...	277	C14H10F3N3	1000444-12-3	14
5	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111622\
Data File : BF131269.D
Acq On : 16 Nov 2022 17:18
Operator : CG\JU
Sample : N5497-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.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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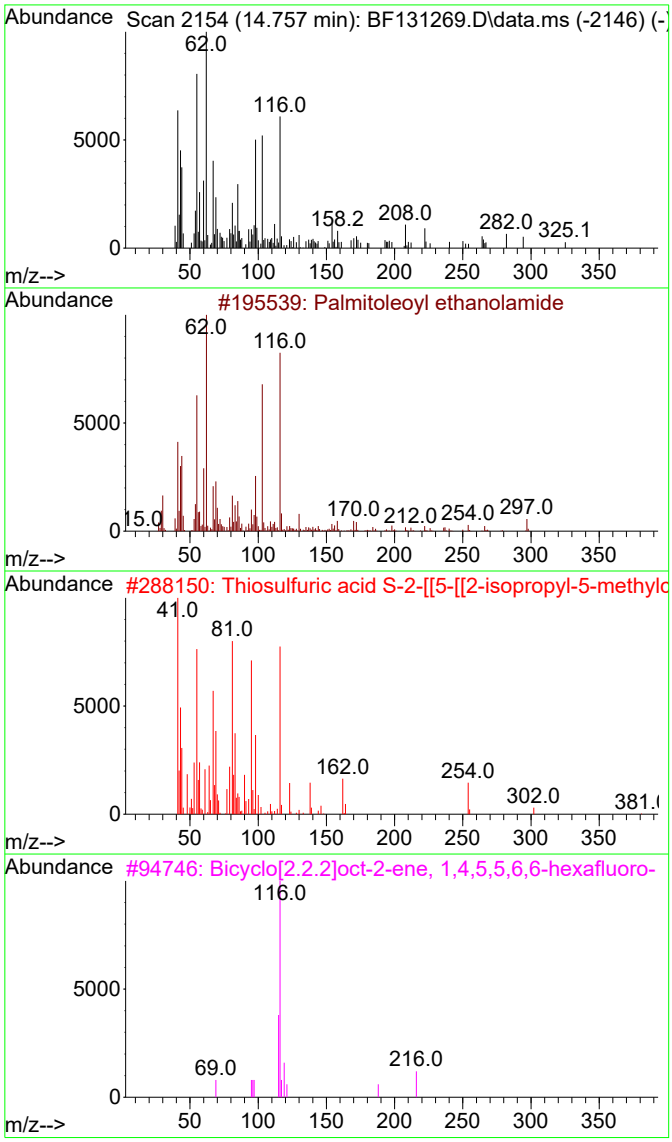
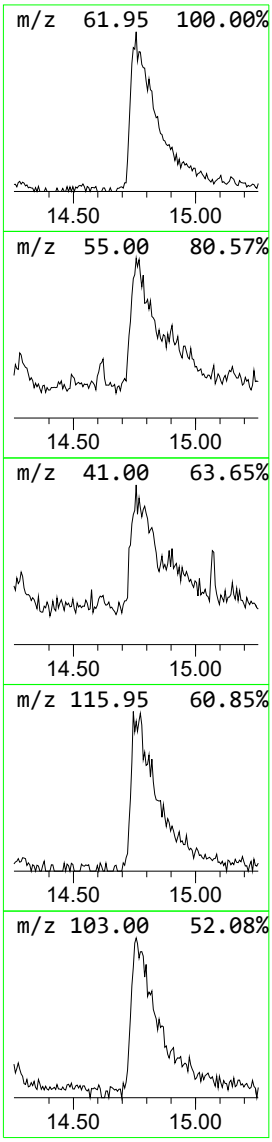
Peak Number 13 Palmitoleoyl ethanolamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	21.85 ng	409201	Chrysene-d12	14.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleoyl ethanolamide	297	C18H35NO2	094421-67-7	64
2	Thiosulfuric acid S-2-[[5-[[2-is...	381	C17H35NO4S2	090392-63-5	9
3	Bicyclo[2.2.2]oct-2-ene, 1,4,5,5...	216	C8H6F6	031463-41-9	9
4	8-Aminodinaphtho[1,2-b:2',3'-d]f...	313	C20H11NO3	112535-18-9	9
5	3-Methylpentane-2,4-diyl dicarba...	204	C8H16N2O4	1000507-43-4	9





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Data File : BF131269.D
Acq On : 16 Nov 2022 17:18
Operator : CG\JU
Sample : N5497-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.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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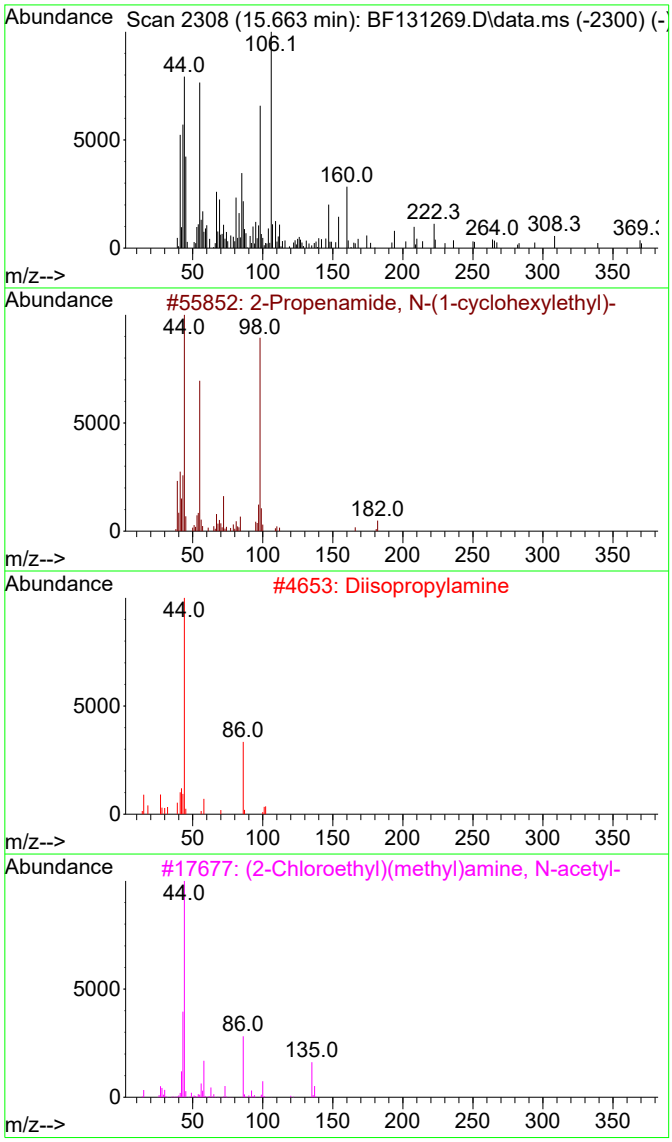
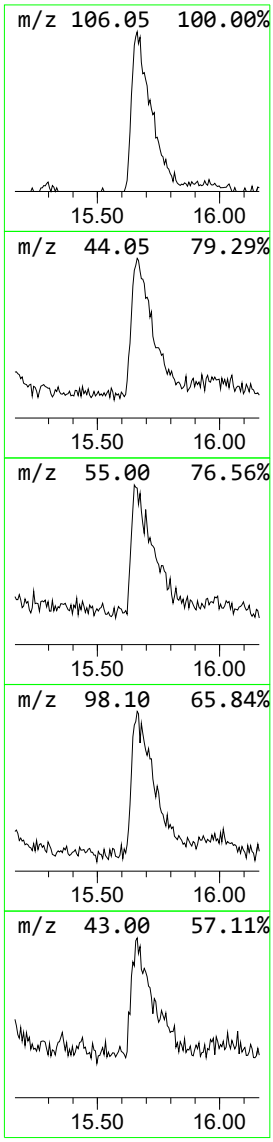
Peak Number 14 unknown15.663 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.663	9.21 ng	271508	Perylene-d12	15.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenamide, N-(1-cyclohexylet...	181	C11H19NO	1000142-14-6	22
2	Diisopropylamine	101	C6H15N	000108-18-9	18
3	(2-Chloroethyl)(methyl)amine, N-...	135	C5H10ClNO	017225-69-3	14
4	Acetamide, N-methyl-N-hexyl-	157	C9H19NO	1000421-40-3	14
5	1-Propyne, 1-(ethenylthio)-	98	C5H6S	058547-36-7	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111622\
Data File : BF131269.D
Acq On : 16 Nov 2022 17:18
Operator : CG\JU
Sample : N5497-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.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
Butane, 2-metho...	2.281	86.1	ng	2159240	1	6.975	501799	20.0
3-Penten-2-one,...	4.581	4.5	ng	113302	1	6.975	501799	20.0
2-Pentanone, 4-...	5.187	11.1	ng	278802	1	6.975	501799	20.0
1-Octanol, 5,7,...	11.157	2.8	ng	94134	4	11.522	680549	20.0
Tridecanoic acid	12.045	2.4	ng	80343	4	11.522	680549	20.0
Linoelaidic acid	12.751	10.2	ng	348343	4	11.522	680549	20.0
9-Octadecenoic ...	12.769	25.1	ng	855051	4	11.522	680549	20.0
Octadecanoic acid	12.839	4.3	ng	146989	4	11.522	680549	20.0
Oxazole, 2-(8Z)...	13.457	8.0	ng	150330	5	14.180	374580	20.0
Carbonic acid, ...	14.092	5.3	ng	100286	5	14.180	374580	20.0
unknown14.280	14.280	3.3	ng	61343	5	14.180	374580	20.0
Palmitoleoyl et...	14.757	21.9	ng	409201	5	14.180	374580	20.0
unknown15.663	15.663	9.2	ng	271508	6	15.727	589881	20.0