LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048047.D
Acq On : 28 Jan 2021 3:42
Operator : CG/JU
Sample : M1226-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0050-044-COMP-D-ELUTRIATE

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_G\METHODS\8270-BG012521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048047.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.676	391	398	412	rVB	563598	902482	26.12%	4.628%
2	7.269	661	669	681	rVB	413633	746042	21.59%	3.826%
3	8.121	808	814	820	rBV	194883	331233	9.59%	1.699%
4	9.284	1004	1012	1022	rVB	519622	930833	26.94%	4.774%
5	10.935	1285	1293	1300	rBV	254614	446184	12.91%	2.288%
6	13.373	1700	1708	1715	rBV	1347925	2088902	60.46%	10.713%
7	13.567	1738	1741	1748	rVB2	24648	37598	1.09%	0.193%
8	14.190	1842	1847	1851	rBV	86013	123917	3.59%	0.635%
9	14.689	1927	1932	1933	rBV	35035	42746	1.24%	0.219%
10	14.742	1933	1941	1952	rVB2	456858	923185	26.72%	4.734%
11	15.142	2004	2009	2017	rBV3	27921	45108	1.31%	0.231%
12	16.229	2187	2194	2202	rBV	1244124	1903771	55.10%	9.763%
13	16.511	2236	2242	2249	rBV2	48325	89184	2.58%	0.457%
14	17.486	2402	2408	2416	rBV	561496	861499	24.93%	4.418%
15	17.762	2448	2455	2461	rBV	570973	716403	20.73%	3.674%
16	18.373	2552	2559	2567	rBV	892502	1259105	36.44%	6.457%
17	18.438	2568	2570	2576	rVB	29702	45605	1.32%	0.234%
18	19.137	2685	2689	2693	rBV	43945	54243	1.57%	0.278%
19	19.490	2745	2749	2751	rBV2	73878	91933	2.66%	0.471%
20	19.513	2751	2753	2760	rVB5	41492	67204	1.94%	0.345%
21	19.637	2769	2774	2784	rBV	791651	1026507	29.71%	5.264%
22	20.089	2845	2851	2861	rVB	2613970	3455281	100.00%	17.720%
23	20.776	2965	2968	2973	rVB	32239	41492	1.20%	0.213%
24	20.882	2982	2986	2991	rVB4	29481	53681	1.55%	0.275%
25	20.988	3001	3004	3009	rVB	109997	142410	4.12%	0.730%
26	21.399	3069	3074	3081	rBV	404403	613035	17.74%	3.144%
27	21.763	3129	3136	3143	rBV	631529	1015230	29.38%	5.206%
28	21.963	3167	3170	3176	rVB4	34754	43409	1.26%	0.223%
29	22.592	3273	3277	3278	rBV3	27735	36601	1.06%	0.188%
30	23.491	3426	3430	3436	rVB	32969	55691	1.61%	0.286%
31	24.120	3535	3537	3543	rVB4	33273	53821	1.56%	0.276%
32	25.048	3686	3695	3712	rVB2	354333	1071125	31.00%	5.493%
33	26.387	3916	3923	3934	rBV7	59695	183994	5.33%	0.944%

Sum of corrected areas: 19499454

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
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Acq On : 28 Jan 2021 3:42
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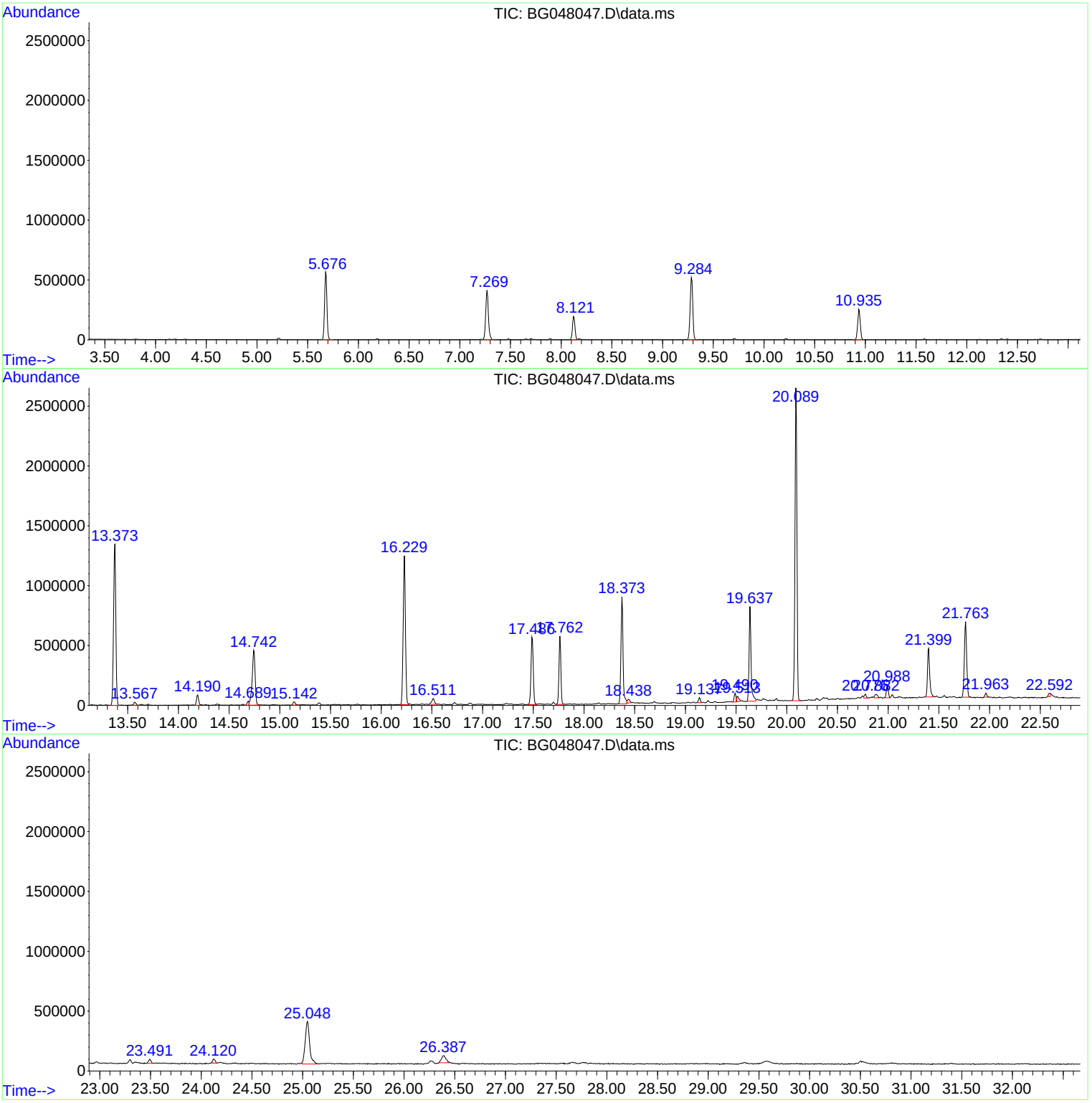
Sample : M1226-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048047.D
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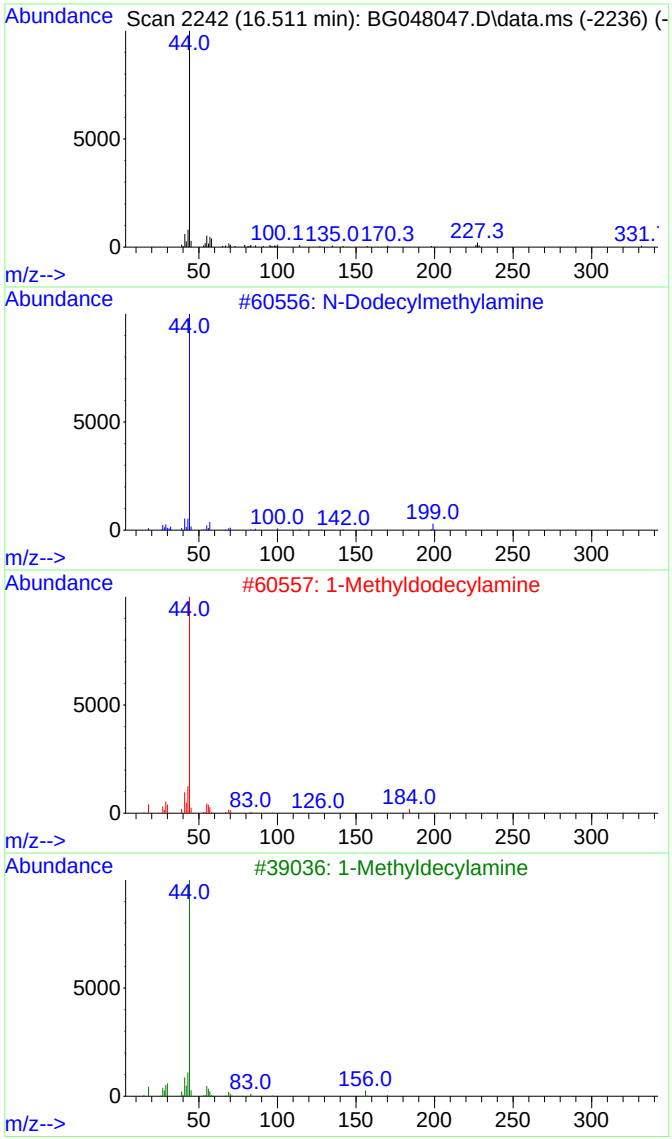
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

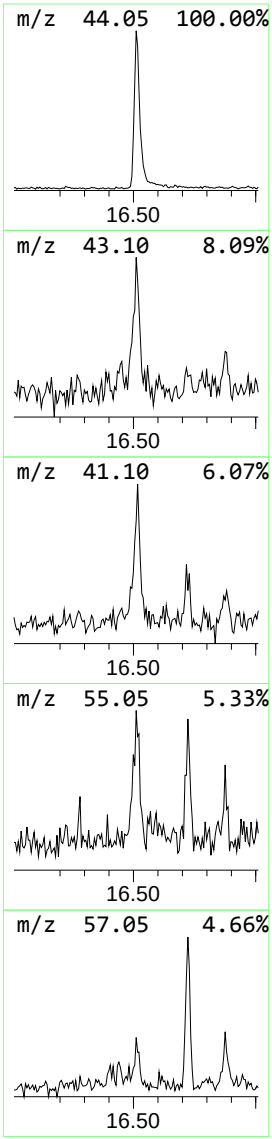
****

Peak Number 1 N-Dodecylmethylamine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.511	2.07 ng	89184	Phenanthrene-d10	17.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Dodecylmethylamine	199	C13H29N	1000342-26-1	56
2	1-Methyldodecylamine	199	C13H29N	013205-57-7	40
3	1-Methyldecylamine	171	C11H25N	013205-56-6	39
4	1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	32
5	12-Methylaminolauric acid	229	C13H27NO2	007408-81-3	9





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Data File : BG048047.D
Acq On : 28 Jan 2021 3:42
Operator : CG/JU
Sample : M1226-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

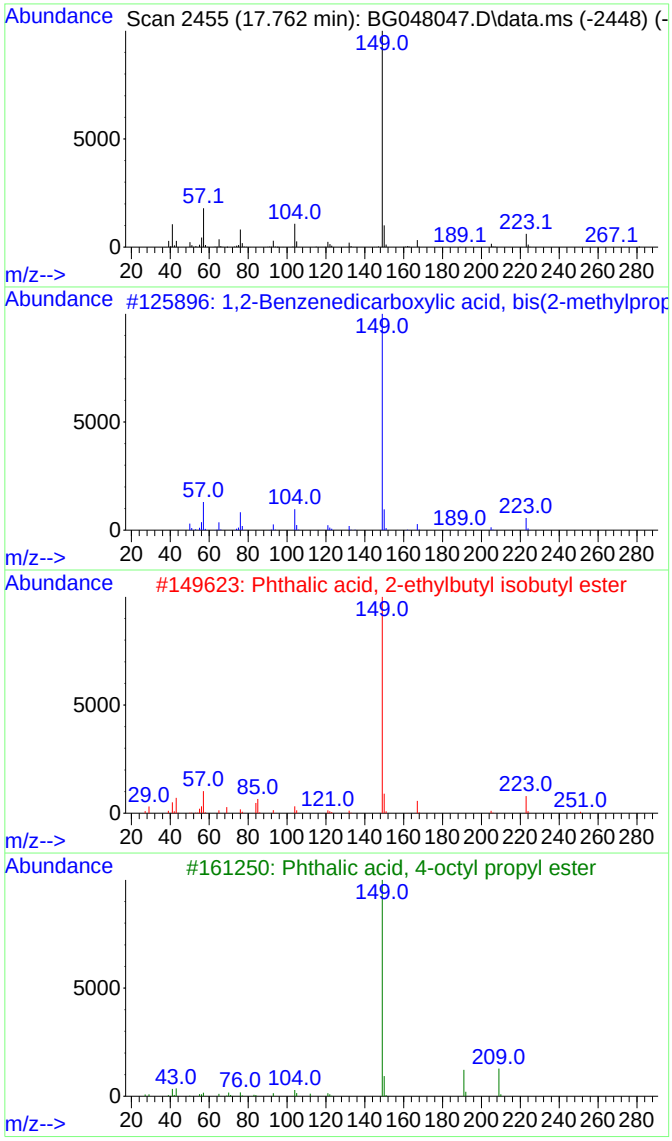
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

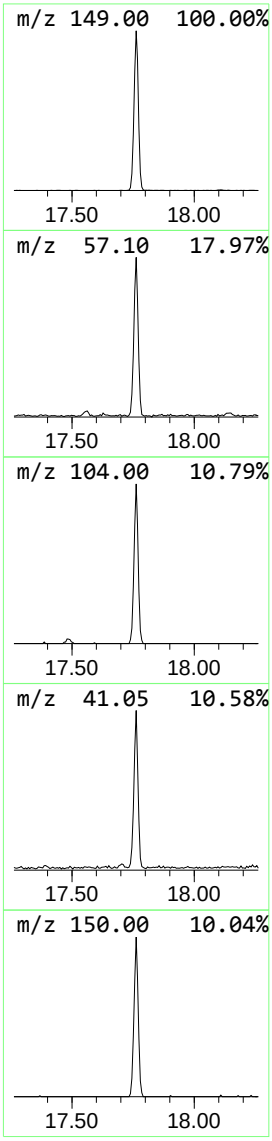
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,2-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.762	16.63 ng	716403	Phenanthrene-d10	17.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2	Phthalic acid, 2-ethylbutyl isob...	306	C18H26O4	1000356-88-9	78
3	Phthalic acid, 4-octyl propyl ester	320	C19H28O4	1000314-83-7	72
4	1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	72
5	Phthalic acid, hexadecyl propyl ...	432	C27H44O4	1000309-06-5	72





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Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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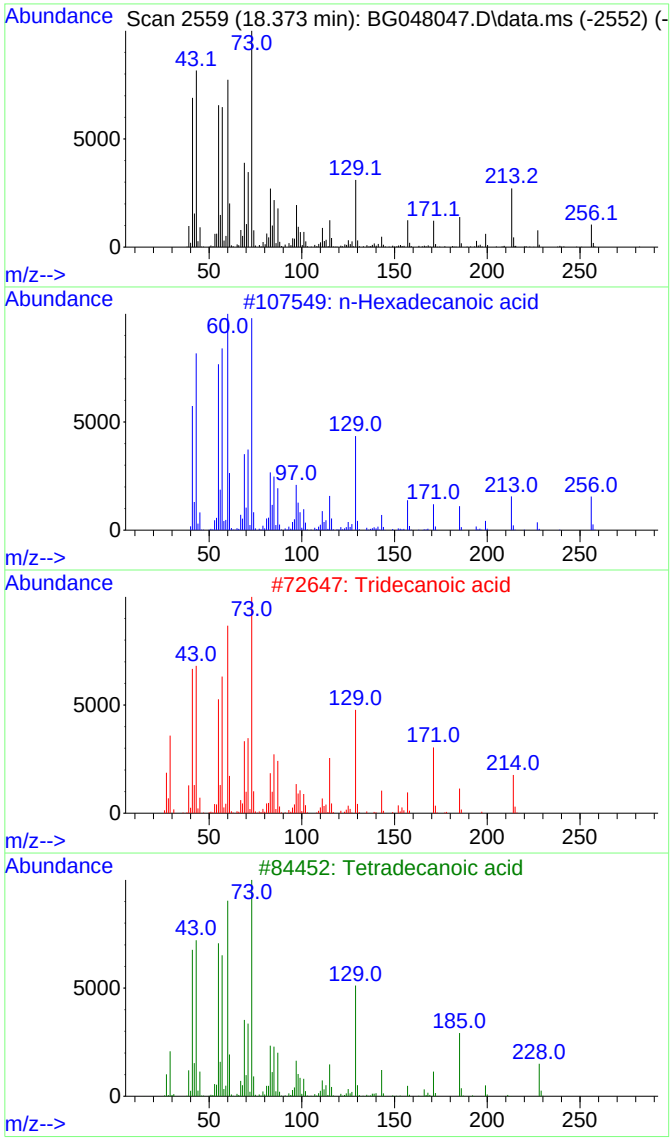
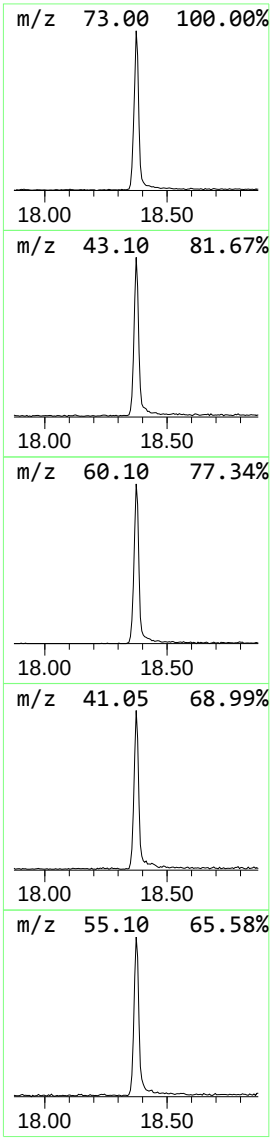
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.373	29.23 ng	1259110	Phenanthrene-d10	17.486

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	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Data File : BG048047.D
Acq On : 28 Jan 2021 3:42
Operator : CG/JU
Sample : M1226-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

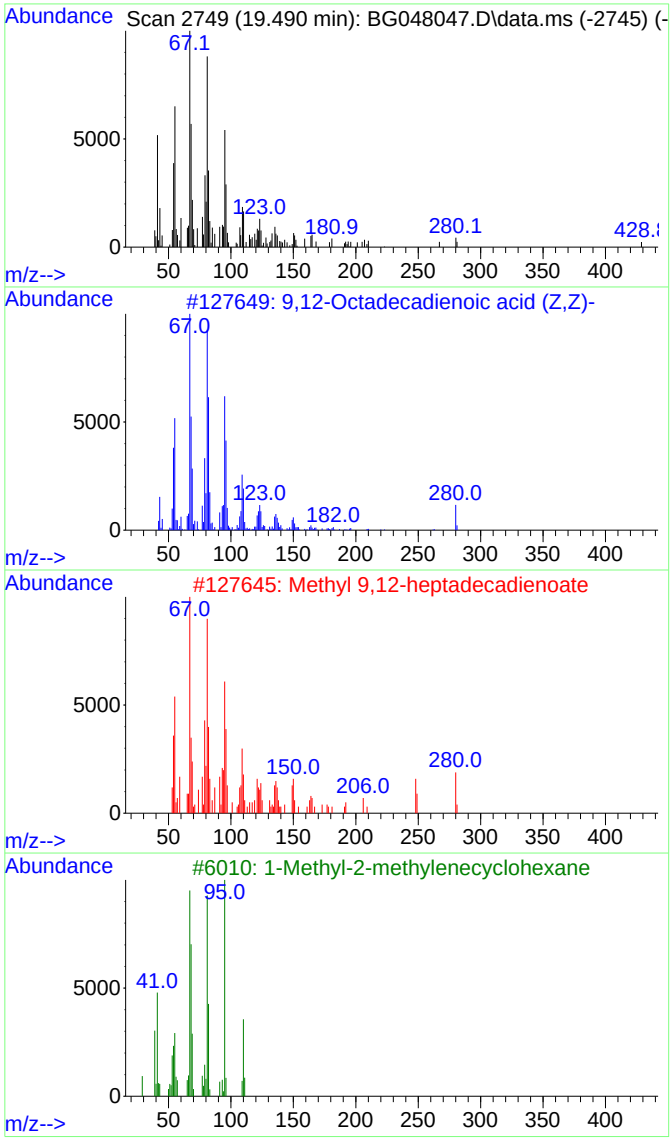
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

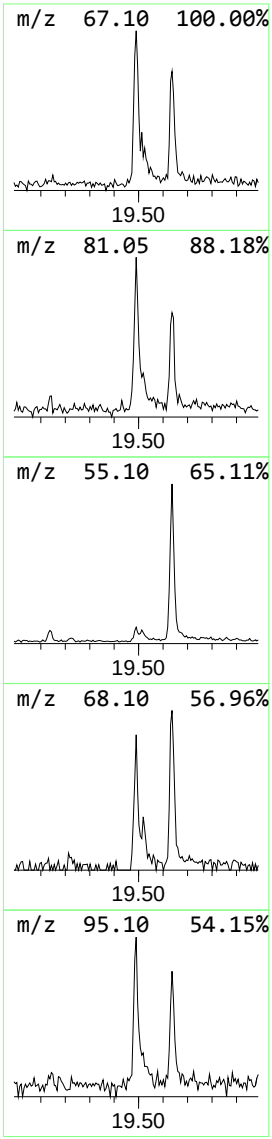
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid (... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.490	2.13 ng	91933	Phenanthrene-d10	17.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	93
2	Methyl 9,12-heptadecadienoate	280	C18H32O2	1000336-36-2	89
3	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	72
4	Norbornane	96	C7H12	000279-23-2	68
5	Bicyclo[4.1.0]heptane, 3-methyl-	110	C8H14	041977-47-3	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
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Sample : M1226-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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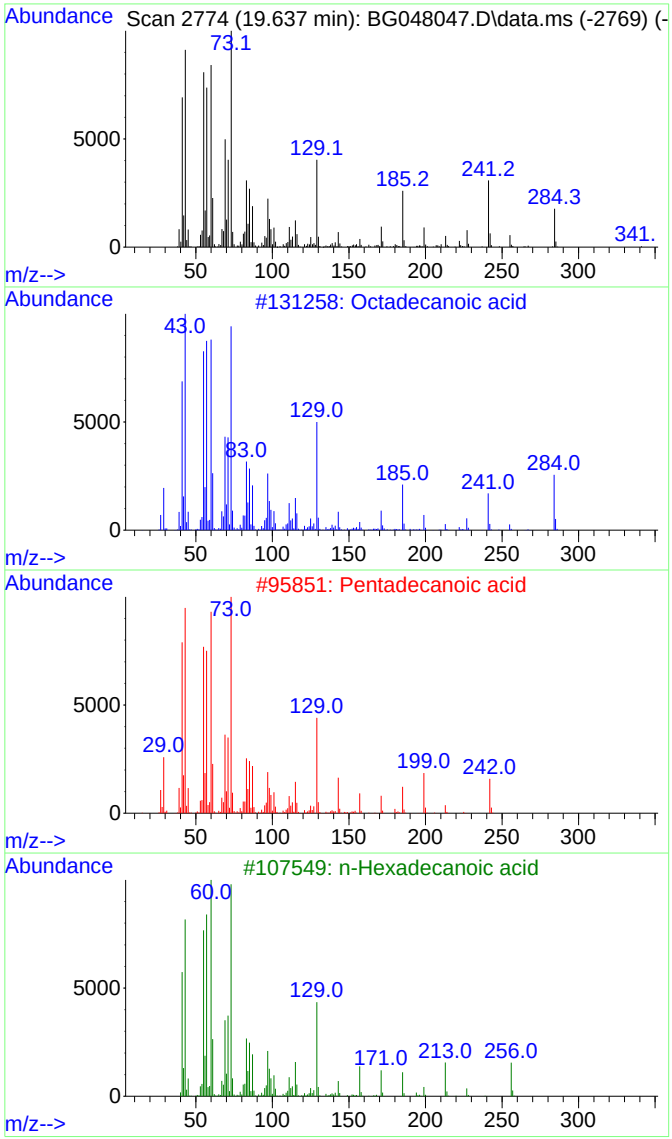
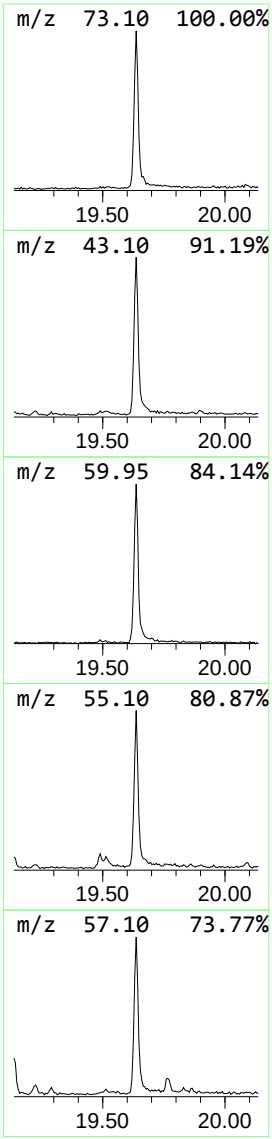
Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.637	20.22 ng	1026510	Chrysene-d12	21.764

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	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





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Sample : M1226-07
Misc :
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Instrument : BNA_G
ClientSampleId : 0050-044-COMP-D-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
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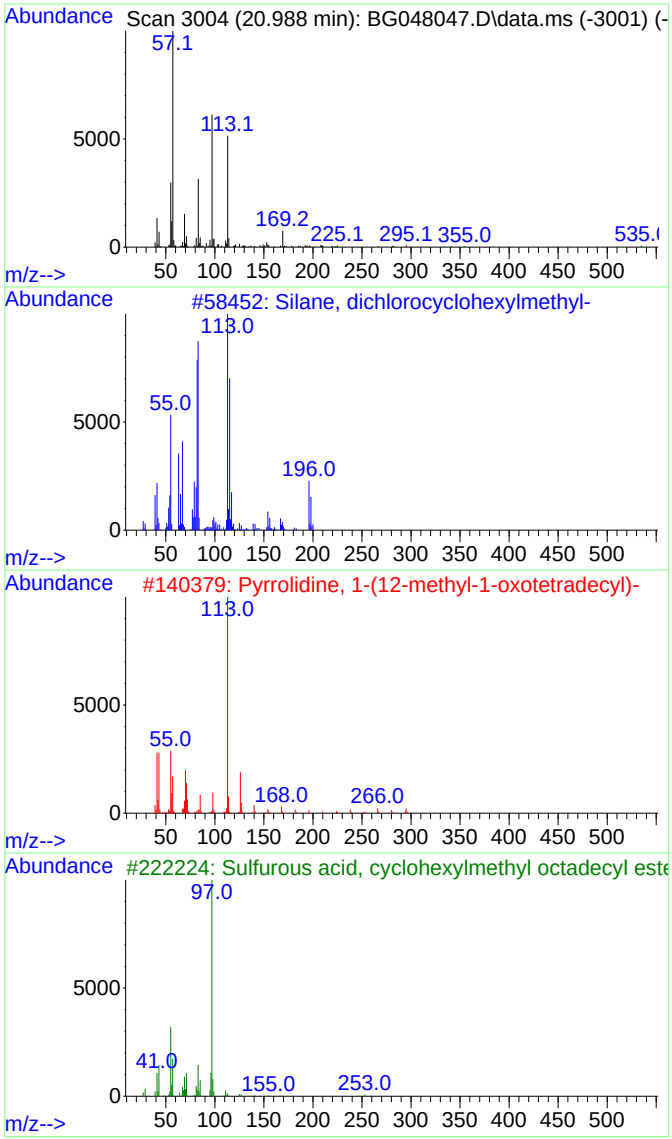
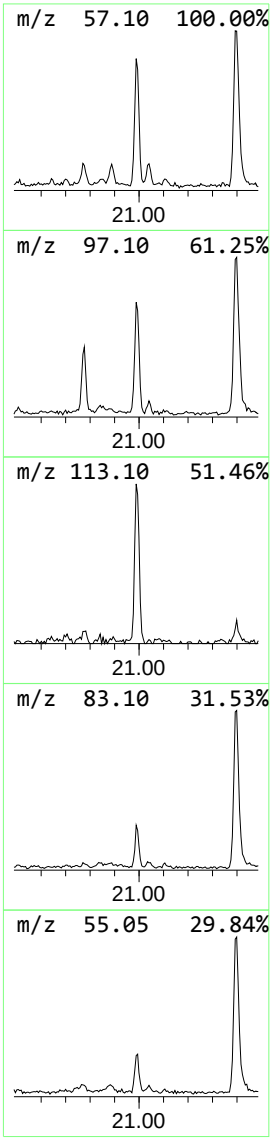
Peak Number 6 unknown20.988 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.988	2.81 ng	142410	Chrysene-d12	21.764

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, dichlorocyclohexylmethyl-	196	C7H14Cl2Si	005578-42-7	38
2	Pyrrolidine, 1-(12-methyl-1-oxot...	295	C19H37NO	056630-61-6	30
3	Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	27
4	N-[4-(Chloro-difluoro-methoxy)-p...	333	C14H18ClF2N3O2	1000296-77-1	27
5	3,4-Methylpropylsuccinimide	155	C8H13NO2	1000248-78-0	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048047.D
Acq On : 28 Jan 2021 3:42
Operator : CG/JU
Sample : M1226-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0050-044-COMP-D-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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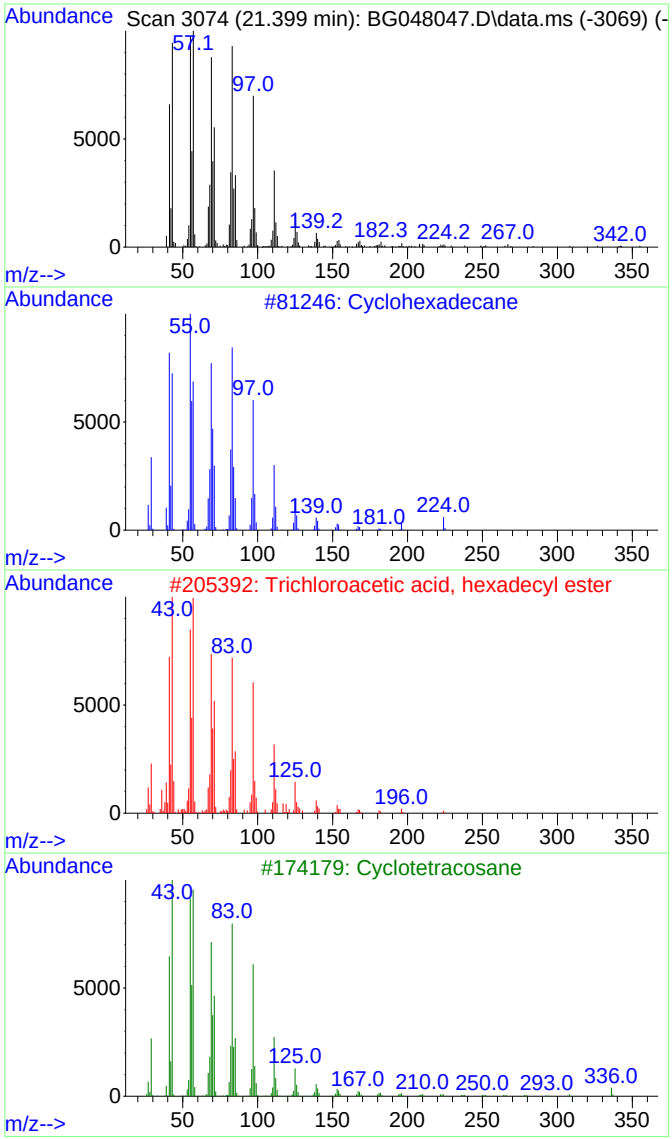
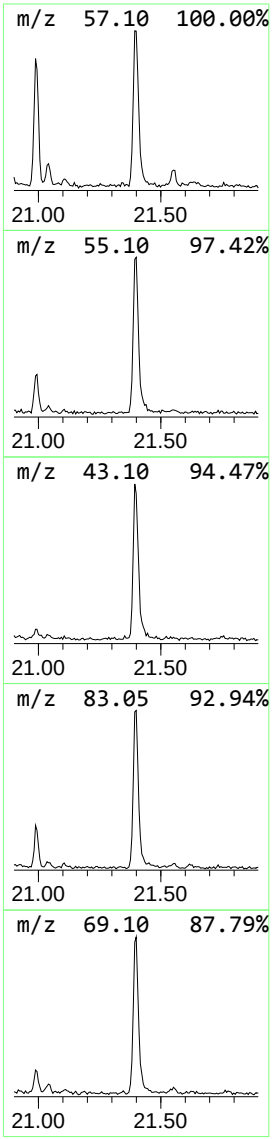
Peak Number 7 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.399	12.08 ng	613035	Chrysene-d12	21.764

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Cyclotetracosane	336	C24H48	000297-03-0	93
4	1-Tricosene	322	C23H46	018835-32-0	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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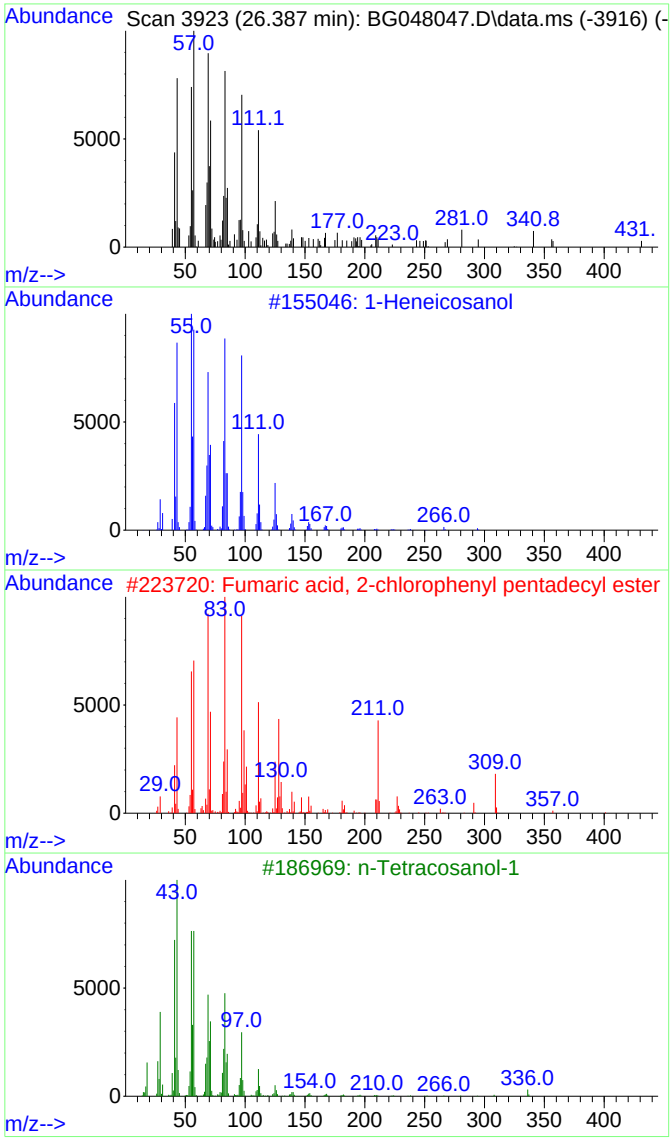
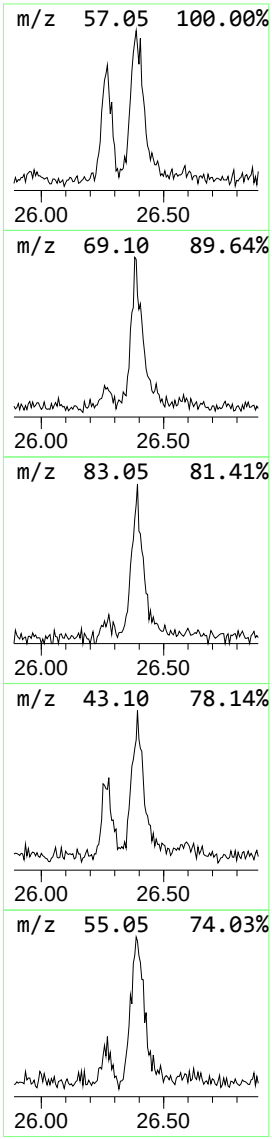
Peak Number 8 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.387	3.44 ng	183994	Perylene-d12	25.048

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	87
2	Fumaric acid, 2-chlorophenyl pen...	436	C25H37ClO4	1000344-83-5	80
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	80
4	Cycloundecane, (1-methylethyl)-	196	C14H28	062338-56-1	78
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	72





Tentatively Identified Compound (LSC) summary

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Data File : BG048047.D
Acq On : 28 Jan 2021 3:42
Operator : CG/JU
Sample : M1226-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0050-044-COMP-D-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
N-Dodecylmethyl...	16.511	2.1	ng	89184	4	17.486	861499	20.0
1,2-Benzenedica...	17.762	16.6	ng	716403	4	17.486	861499	20.0
n-Hexadecanoic ...	18.373	29.2	ng	1259110	4	17.486	861499	20.0
9,12-Octadecadi...	19.490	2.1	ng	91933	4	17.486	861499	20.0
Octadecanoic acid	19.637	20.2	ng	1026510	5	21.764	1015230	20.0
unknown20.988	20.988	2.8	ng	142410	5	21.764	1015230	20.0
Cyclohexadecane	21.399	12.1	ng	613035	5	21.764	1015230	20.0
1-Heneicosanol	26.387	3.4	ng	183994	6	25.048	1071130	20.0