LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041621\
Data File : BG048727.D
Acq On : 16 Apr 2021 16:43
Operator : CG/JU
Sample : M1998-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EB_04-08-2021_SO

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-BG041421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048727.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.629	382	390	399	rBV	178209	294669	14.85%	4.011%
2	7.239	655	664	674	rBV	119986	199319	10.05%	2.713%
3	8.079	801	807	814	rBV3	79588	130512	6.58%	1.776%
4	9.254	999	1007	1017	rBV	300460	521805	26.30%	7.102%
5	10.911	1281	1289	1295	rVB	101201	175208	8.83%	2.385%
6	13.355	1698	1705	1712	rBV	772231	1161627	58.55%	15.811%
7	14.736	1934	1940	1947	rVB	154657	240887	12.14%	3.279%
8	16.229	2189	2194	2203	rBV	615504	949490	47.86%	12.924%
9	17.492	2402	2409	2416	rBV	219917	331168	16.69%	4.508%
10	18.379	2555	2560	2565	rBV3	23964	33859	1.71%	0.461%
11	18.579	2588	2594	2597	rBV6	12509	28450	1.43%	0.387%
12	18.661	2605	2608	2612	rVB4	17067	22182	1.12%	0.302%
13	19.807	2791	2803	2804	rBV8	35565	81609	4.11%	1.111%
14	20.106	2847	2854	2861	rVB	1553057	1984040	100.00%	27.005%
15	20.841	2968	2979	2986	rBV5	43751	126727	6.39%	1.725%
16	21.411	3072	3076	3086	rVB6	39871	82501	4.16%	1.123%
17	21.505	3087	3092	3099	rVB	24588	39927	2.01%	0.543%
18	21.793	3134	3141	3152	rVB	228945	385905	19.45%	5.253%
19	22.451	3243	3253	3263	rBV6	32070	117743	5.93%	1.603%
20	23.802	3476	3483	3484	rBV7	20484	36102	1.82%	0.491%
21	23.820	3484	3486	3489	rVV4	15289	21261	1.07%	0.289%
22	24.431	3582	3590	3592	rBV5	12703	27146	1.37%	0.369%
23	25.136	3701	3710	3719	rBV3	122375	354687	17.88%	4.828%

Sum of corrected areas: 7346824

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Misc :
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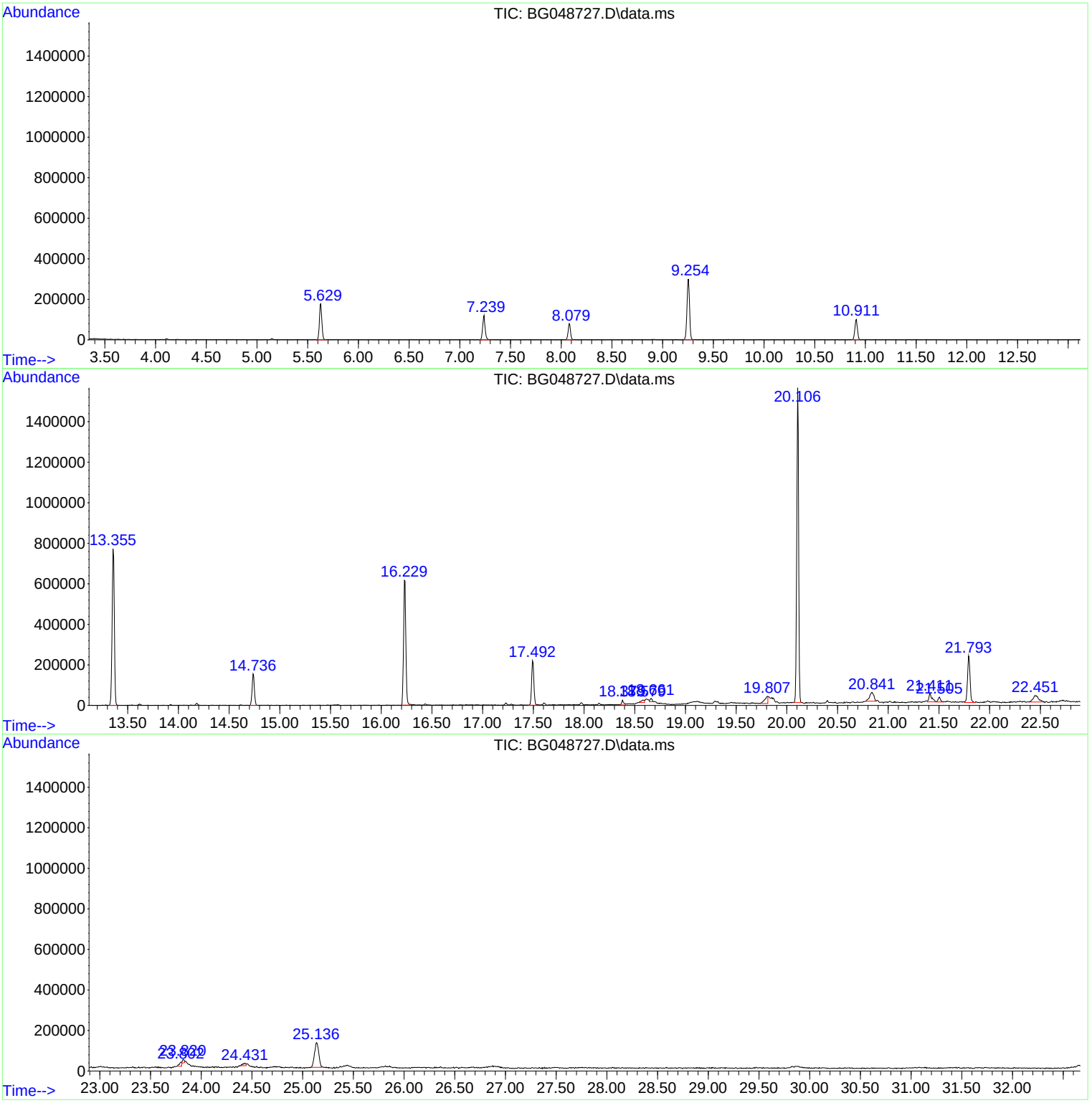
Instrument :
BNA_G
ClientSampleId :
EB_04-08-2021_SO

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.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 : BG048727.D
Acq On : 16 Apr 2021 16:43
Operator : CG/JU
Sample : M1998-13
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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

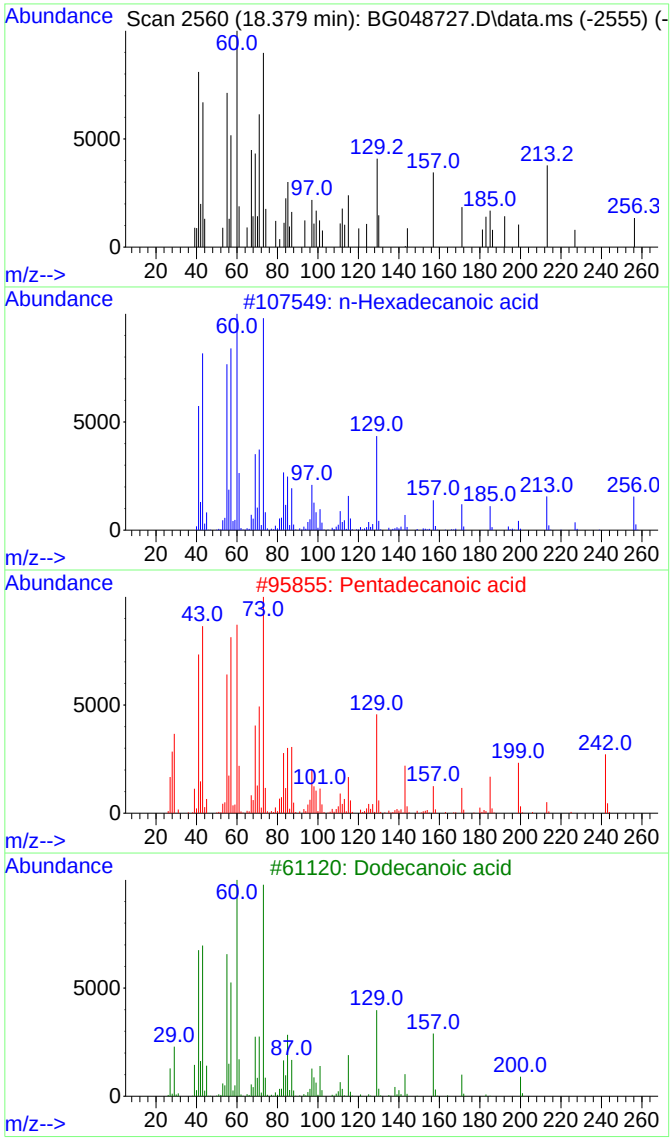
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

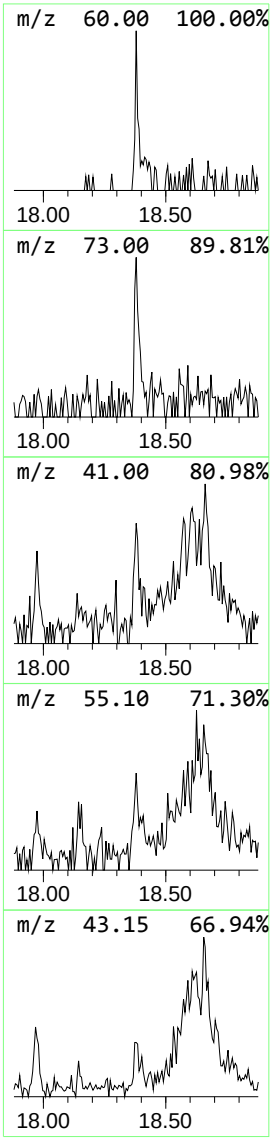
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.379	2.04 ng	33859	Phenanthrene-d10	17.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	53
5	Tridecanoic acid	214	C13H26O2	000638-53-9	50





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Acq On : 16 Apr 2021 16:43
Operator : CG/JU
Sample : M1998-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB_04-08-2021_SO

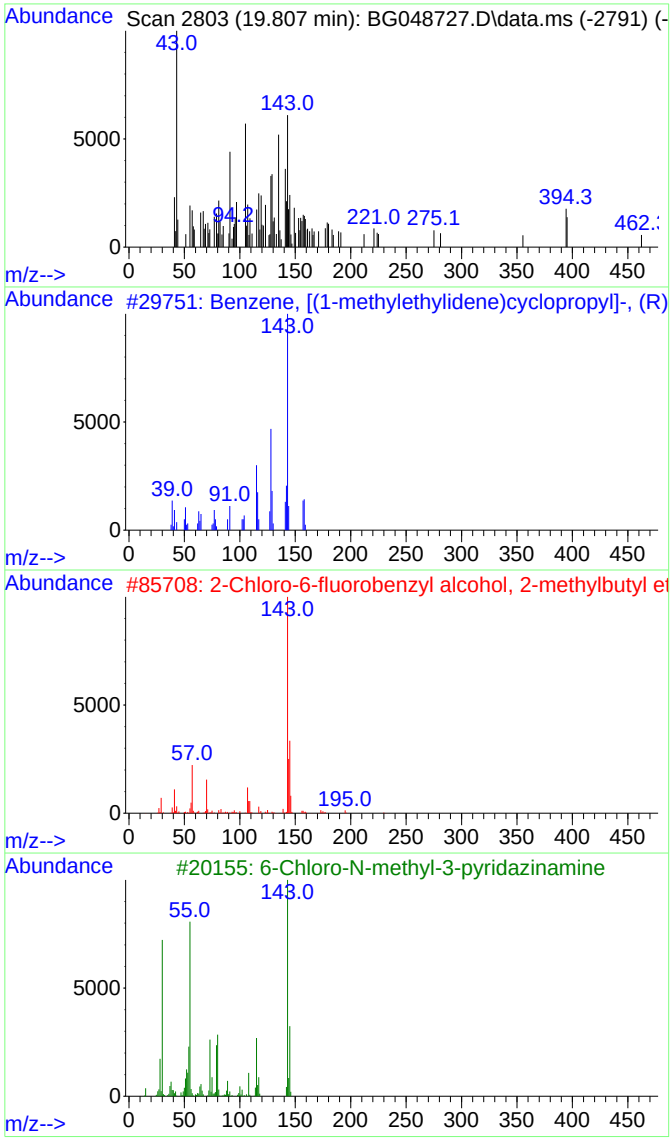
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

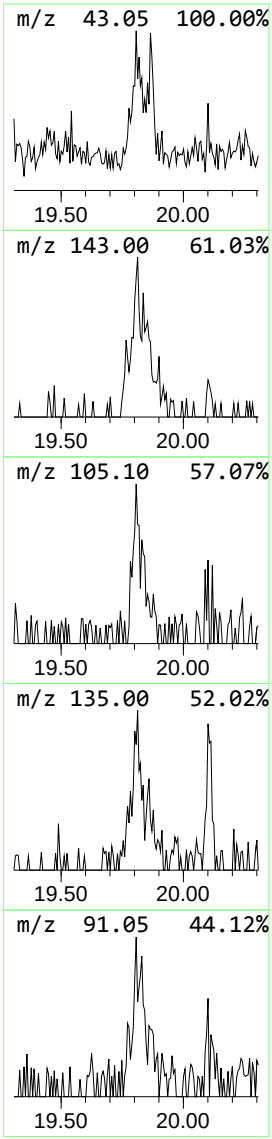
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, [(1-methylethylide... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.807	4.23 ng	81609	Chrysene-d12	21.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, [(1-methylethylidene)cy...	158	C12H14	024524-55-8	18
2	2-Chloro-6-fluorobenzyl alcohol,...	230	C12H16ClFO	1000378-14-8	14
3	6-Chloro-N-methyl-3-pyridazinamine	143	C5H6ClN3	014959-32-1	14
4	3-Chloro-2-fluorobenzyl bromide	222	C7H5BrClF	085070-47-9	14
5	(1-Methylenepent-2-enyl)benzene	158	C12H14	084313-24-6	14





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Data File : BG048727.D
Acq On : 16 Apr 2021 16:43
Operator : CG/JU
Sample : M1998-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EB_04-08-2021_SO

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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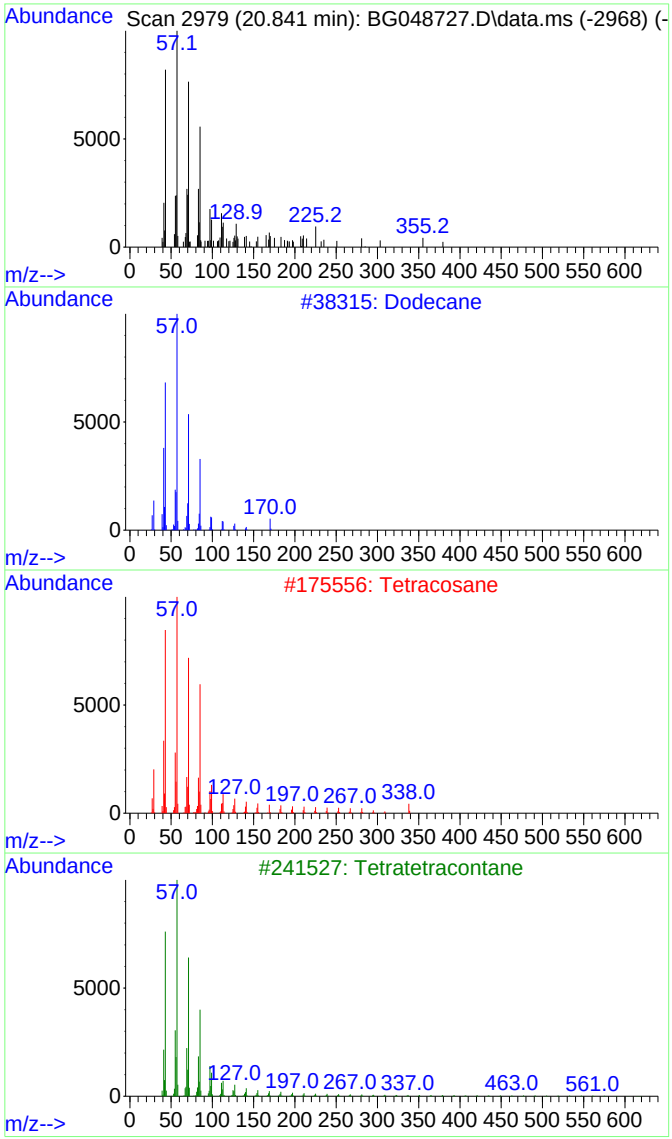
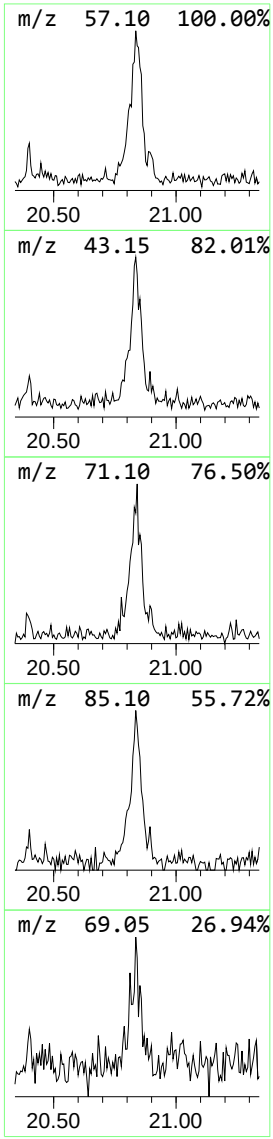
Peak Number 3 Dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.841	6.57 ng	126727	Chrysene-d12	21.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	76
2	Tetracosane	338	C24H50	000646-31-1	64
3	Tetratetracontane	619	C44H90	007098-22-8	58
4	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	58
5	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	58





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Acq On : 16 Apr 2021 16:43
Operator : CG/JU
Sample : M1998-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EB_04-08-2021_SO

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

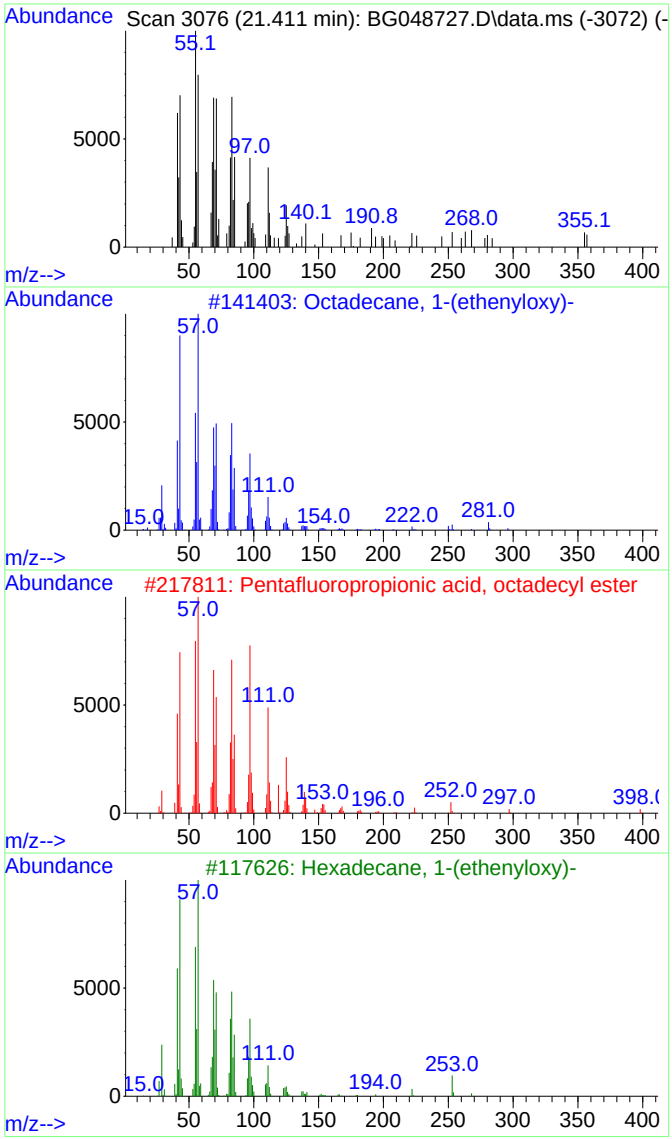
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

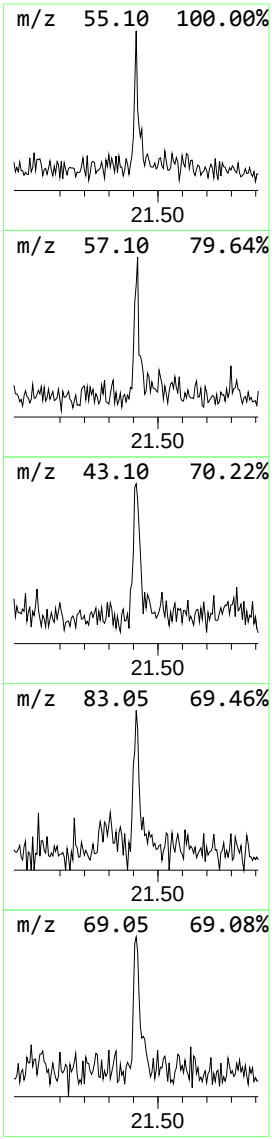
****

Peak Number 4 Octadecane, 1-(ethenyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.411	4.28 ng	82501	Chrysene-d12	21.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	80
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	72
3	Hexadecane, 1-(ethenyloxy)-	268	C18H36O	000822-28-6	64
4	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	64
5	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	58





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Data File : BG048727.D
Acq On : 16 Apr 2021 16:43
Operator : CG/JU
Sample : M1998-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EB_04-08-2021_SO

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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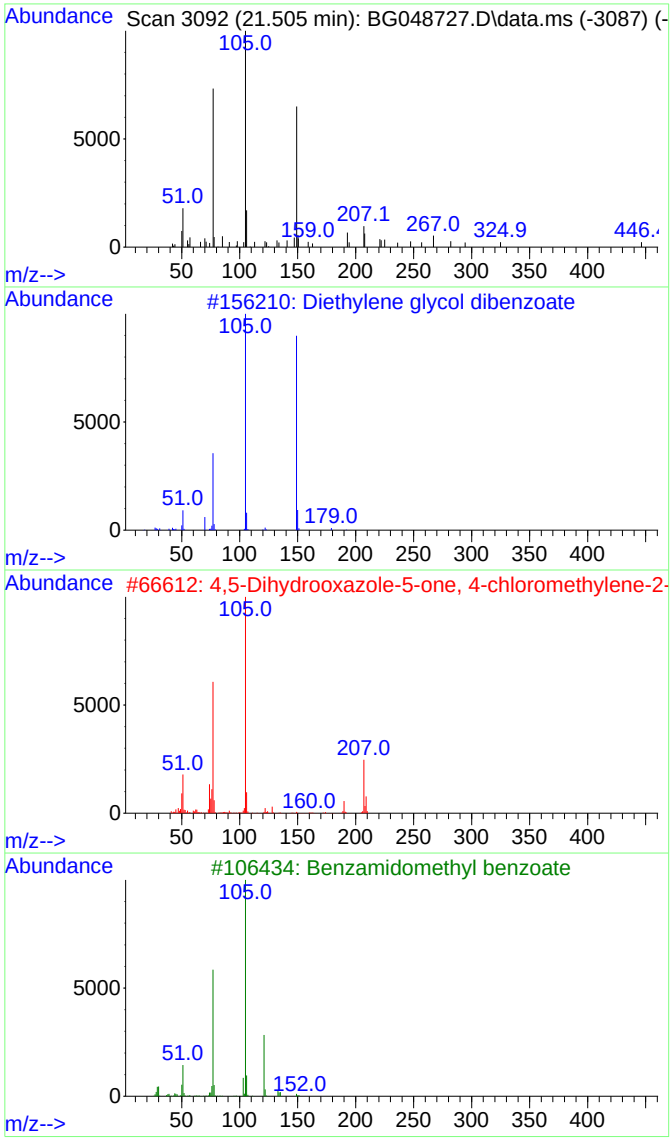
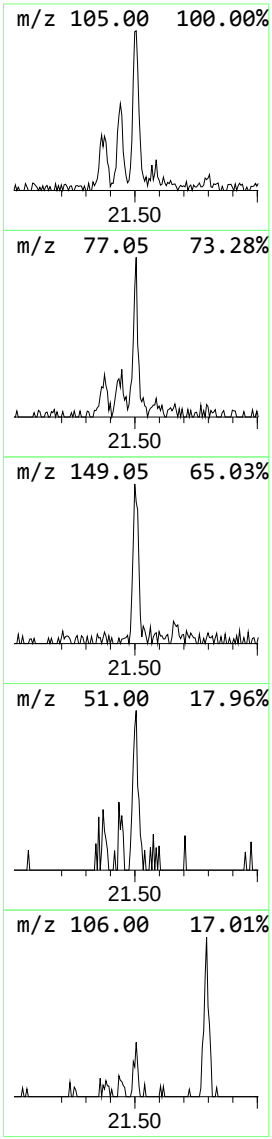
Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.505	2.07 ng	39927	Chrysene-d12	21.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2	4,5-Dihydrooxazole-5-one, 4-chlo...	207	C10H6ClNO2	014848-36-3	50
3	Benzamidomethyl benzoate	255	C15H13NO3	061652-83-3	47
4	Glyoxylamide, N,2-diphenyl-	225	C14H11NO2	004732-66-5	47
5	Benzofurazan-5-carbohydrazide, N...	282	C14H10N4O3	1000272-94-4	43





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Sample : M1998-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EB_04-08-2021_SO

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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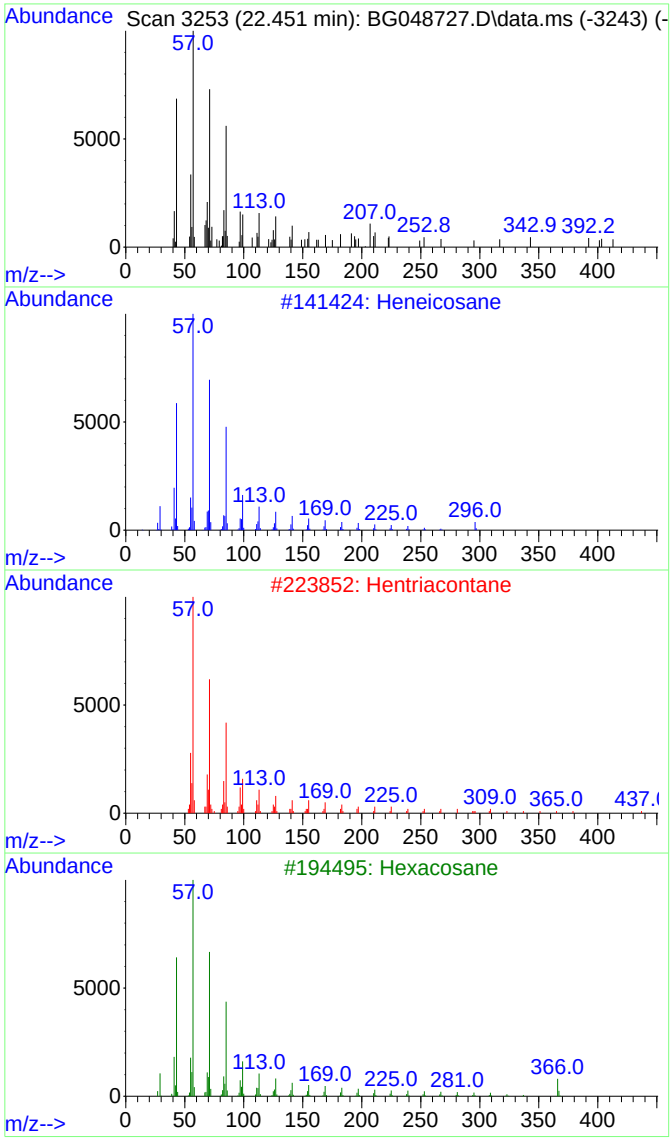
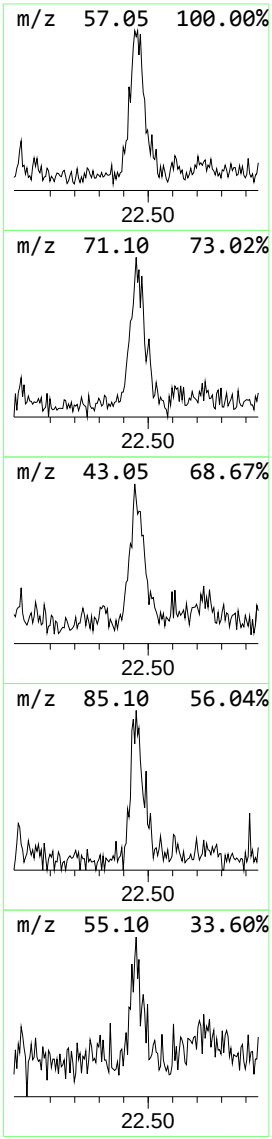
****

Peak Number 6 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.451	6.10 ng	117743	Chrysene-d12	21.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	58
2	Hentriacontane	437	C31H64	000630-04-6	58
3	Hexacosane	366	C26H54	000630-01-3	58
4	Eicosane	282	C20H42	000112-95-8	58
5	Tetracosane	338	C24H50	000646-31-1	58





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Misc :
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Instrument :
BNA_G
ClientSampleId :
EB_04-08-2021_SO

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.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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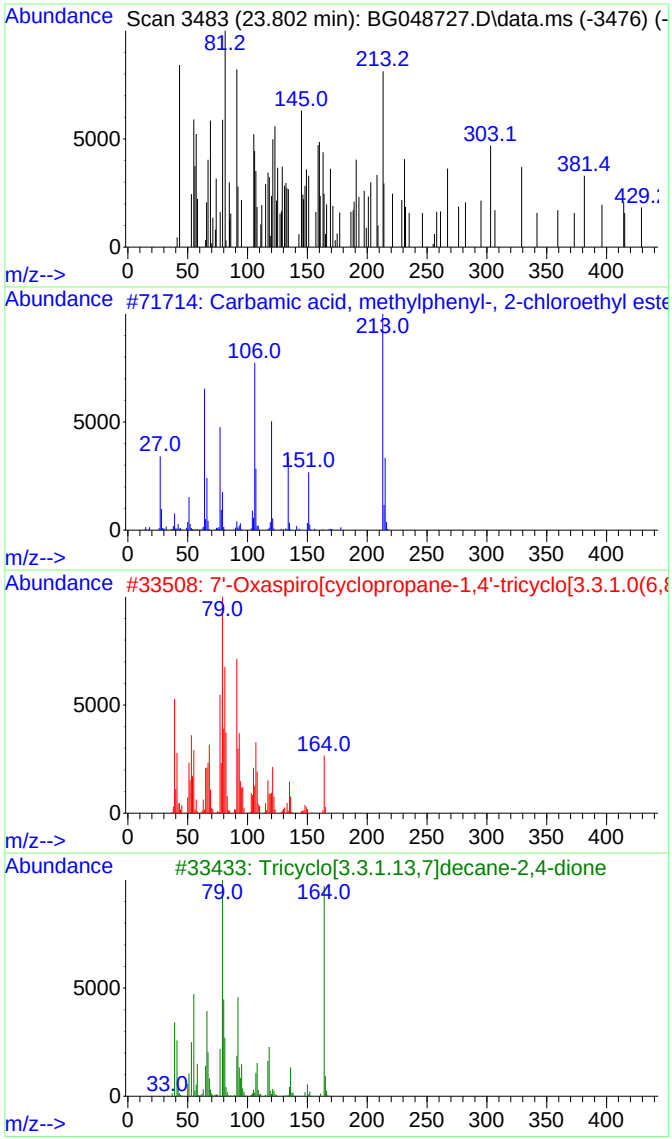
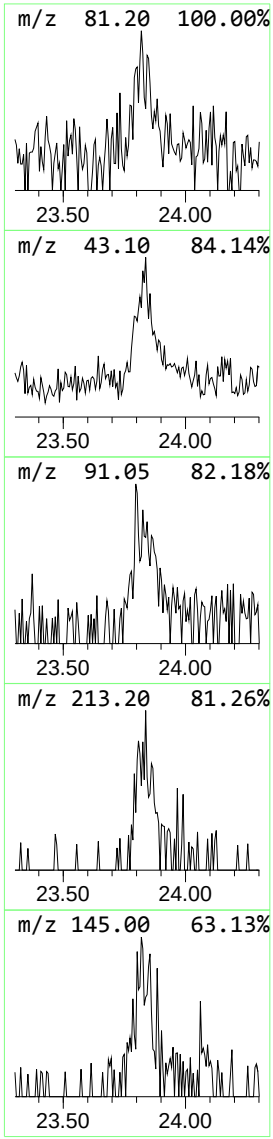
Peak Number 7 unknown23.802 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.802	2.04 ng	36102	Perylene-d12	25.136

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbamic acid, methylphenyl-, 2-...	213	C10H12ClNO2	055030-68-7	23
2	7'-Oxaspiro[cyclopropane-1,4'-tr...	164	C10H12O2	109637-57-2	10
3	Tricyclo[3.3.1.13,7]decane-2,4-d...	164	C10H12O2	019214-00-7	10
4	Anthranilic acid, N-(o-fluorophe...	231	C13H10FNO2	000054-58-0	10
5	Pyridine-2-carboxylic acid, (2-a...	213	C12H11N3O	1000317-79-6	10





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	18.379	2.0	ng	33859	4	17.492	331168	20.0
Benzene, [(1-me...	19.807	4.2	ng	81609	5	21.793	385905	20.0
Dodecane	20.841	6.6	ng	126727	5	21.793	385905	20.0
Octadecane, 1-(...	21.411	4.3	ng	82501	5	21.793	385905	20.0
Diethylene glyc...	21.505	2.1	ng	39927	5	21.793	385905	20.0
Heneicosane	22.451	6.1	ng	117743	5	21.793	385905	20.0
unknown23.802	23.802	2.0	ng	36102	6	25.136	354687	20.0