LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

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-BG051520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.543	410	418	434	rBV	663293	1144197	37.86%	4.599%
2	7.152	684	692	705	rBV	745838	1321166	43.71%	5.311%
3	7.951	821	828	837	rBV	264140	466742	15.44%	1.876%
4	8.280	875	884	892	rBV	669737	1219263	40.34%	4.901%
5	9.115	1015	1026	1036	rBV	517556	962017	31.83%	3.867%
6	10.759	1297	1306	1320	rBV	356352	674458	22.32%	2.711%
7	12.410	1580	1587	1594	rBV4	11560	30814	1.02%	0.124%
8	13.221	1716	1725	1734	rBV	1494836	2423171	80.17%	9.741%
9	14.049	1860	1866	1871	rBV	204081	310525	10.27%	1.248%
10	14.595	1949	1959	1967	rBV2	581487	969029	32.06%	3.895%
11	16.093	2207	2214	2222	rBV	1145800	1828377	60.49%	7.350%
12	17.245	2407	2410	2415	rBV6	18318	32178	1.06%	0.129%
13	17.345	2419	2427	2432	rVV	670997	1079753	35.72%	4.340%
14	17.386	2432	2434	2440	rVB	118252	162302	5.37%	0.652%
15	17.480	2446	2450	2456	rVB	22536	30577	1.01%	0.123%
16	18.132	2557	2561	2566	rBV4	50035	79686	2.64%	0.320%
17	18.255	2574	2582	2590	rVB6	50356	134569	4.45%	0.541%
18	18.420	2605	2610	2614	rBV2	38413	74491	2.46%	0.299%
19	19.218	2742	2746	2749	rBV3	67189	77534	2.57%	0.312%
20	19.271	2752	2755	2760	rVB5	25350	43124	1.43%	0.173%
21	19.342	2763	2767	2771	rVV	138711	189177	6.26%	0.760%
22	19.401	2772	2777	2784	rVB	343003	482076	15.95%	1.938%
23	19.759	2830	2838	2845	rVB	314531	569821	18.85%	2.291%
24	19.912	2861	2864	2867	rBV3	49708	62219	2.06%	0.250%
25	19.959	2867	2872	2879	rVV	2181241	3022405	100.00%	12.149%
26	20.446	2952	2955	2959	rVB2	86289	95006	3.14%	0.382%
27	20.946	3037	3040	3047	rVB4	79721	100392	3.32%	0.404%
28	21.263	3090	3094	3101	rVB3	210203	339232	11.22%	1.364%
29	21.603	3145	3152	3157	rBV3	658414	1278894	42.31%	5.141%
30	21.650	3157	3160	3169	rVB	151822	256472	8.49%	1.031%
31	22.408	3285	3289	3298	rVB5	102336	280772	9.29%	1.129%
32	23.419	3457	3461	3470	rVB5	122656	255632	8.46%	1.028%
33	23.765	3514	3520	3527	rBV2	115768	321575	10.64%	1.293%
34	23.871	3533	3538	3543	rBV2	200575	388537	12.86%	1.562%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

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-BG051520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.930	3544	3548	3556	rVB3	175227	366410	12.12%	1.473%
36	24.758	3681	3689	3708	rVB3	357989	1093564	36.18%	4.396%
37	25.298	3776	3781	3790	rVB5	132151	346278	11.46%	1.392%
38	25.909	3875	3885	3894	rVB2	598947	1791015	59.26%	7.199%
39	26.021	3897	3904	3917	rVB4	182017	573624	18.98%	2.306%

Sum of corrected areas: 24877074

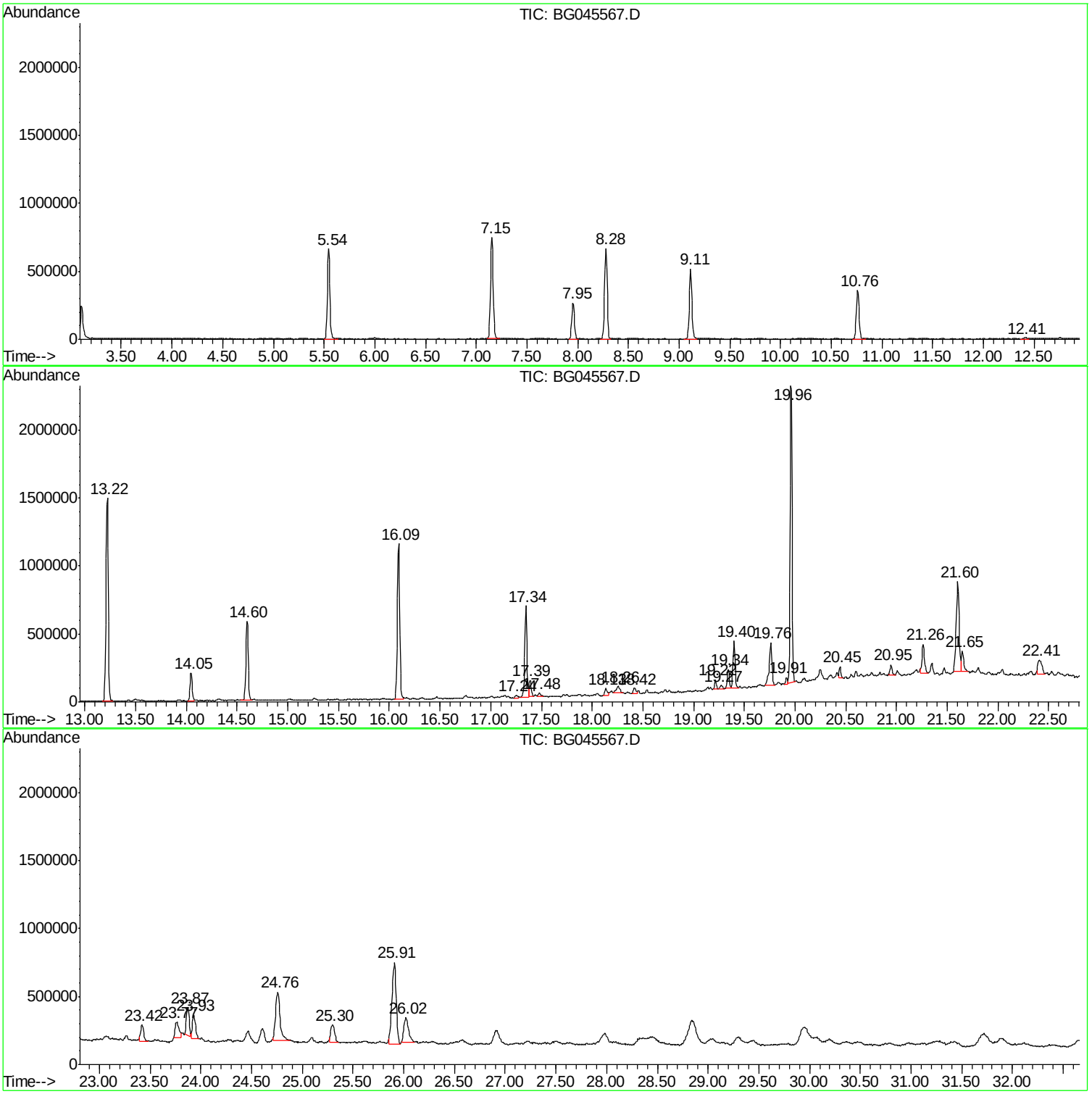
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.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\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

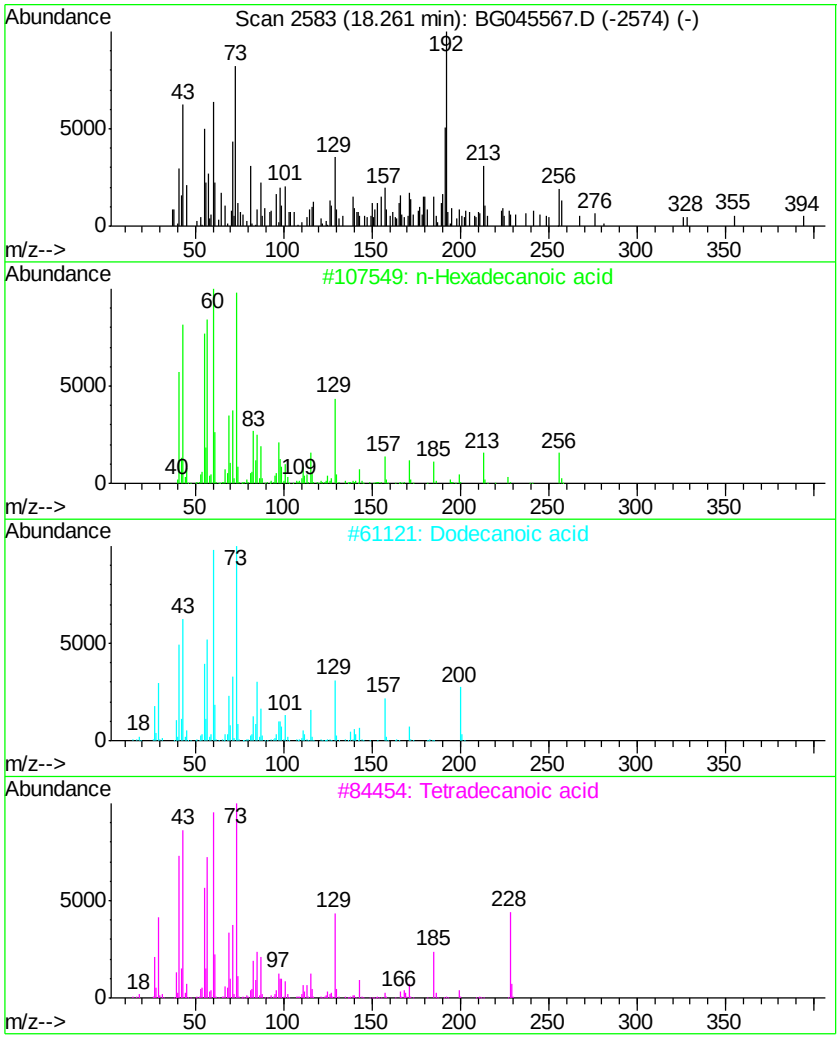
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

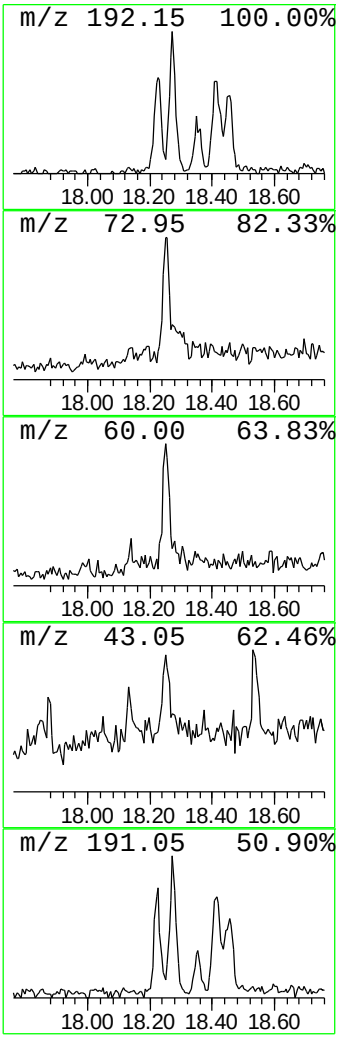
****

Peak Number 2 unknown18.26 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	2.49 ng	134569	Phenanthrene-d10	17.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
2	Dodecanoic acid	200	C12H24O2	000143-07-7	46
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
4	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	35
5	Maltose	342	C12H22O11	000069-79-4	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

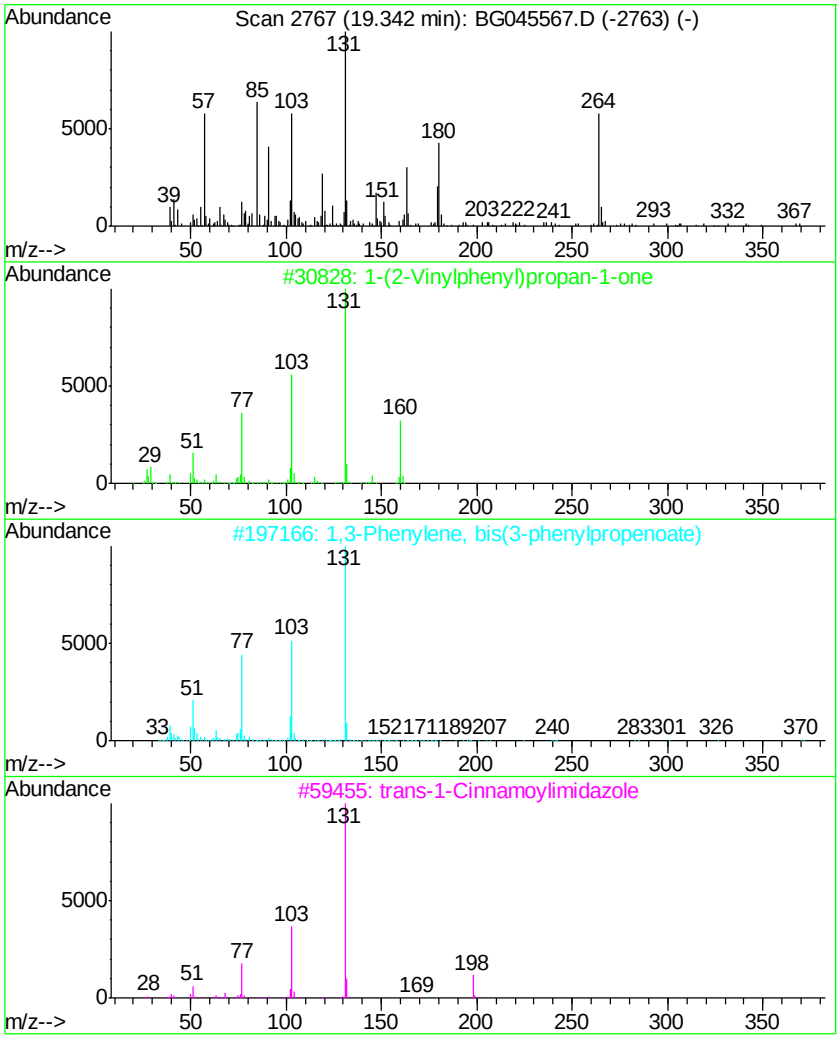
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

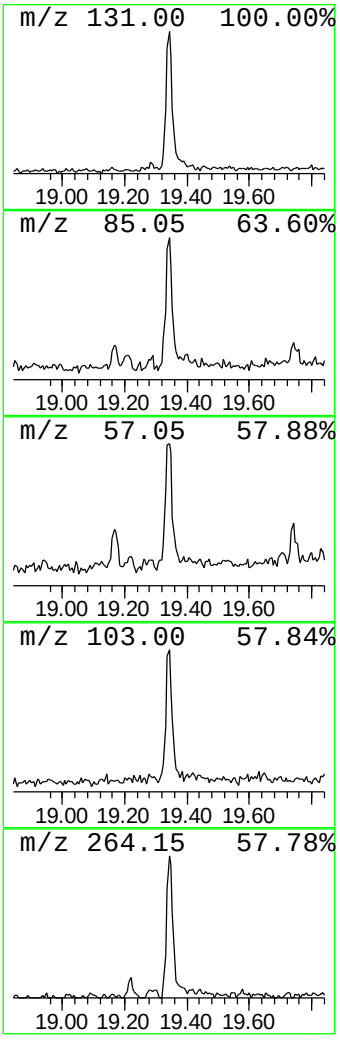
****

Peak Number 3 unknown19.34 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	3.50 ng	189177	Phenanthrene-d10	17.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Vinylphenyl)propan-1-one	160	C11H12O	052095-41-7	22
2	1,3-Phenylene, bis(3-phenylprope...	370	C24H18O4	1000259-62-4	22
3	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	22
4	2-Propenoyl chloride, 3-phenyl-	166	C9H7ClO	000102-92-1	22
5	Cinnamamide, N-(2-thiazolyl)-	230	C12H10N2OS	300829-00-9	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

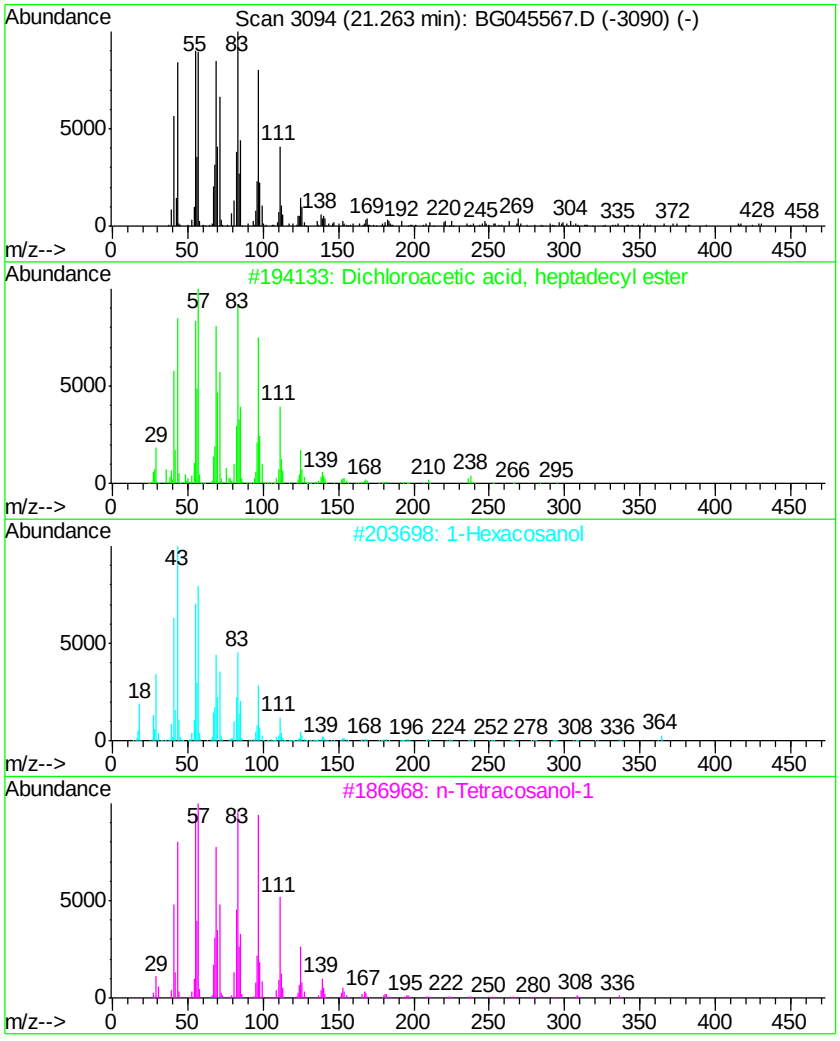
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

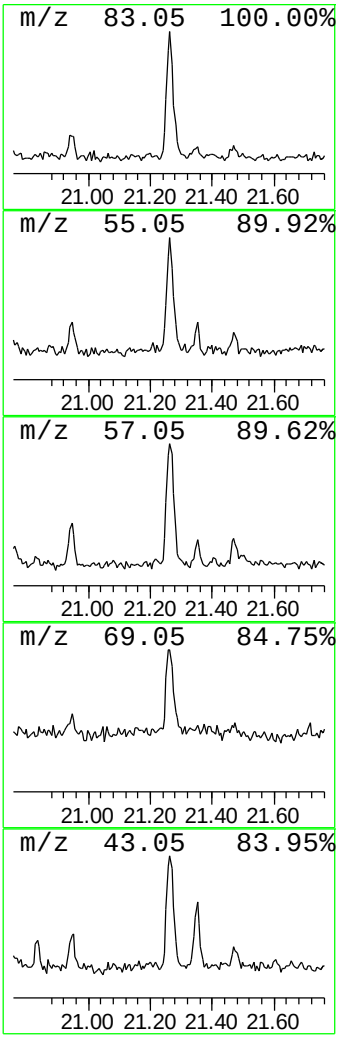
****

Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.26	5.31 ng	339232	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
2	1-Hexacosanol	382	C26H54O	000506-52-5	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

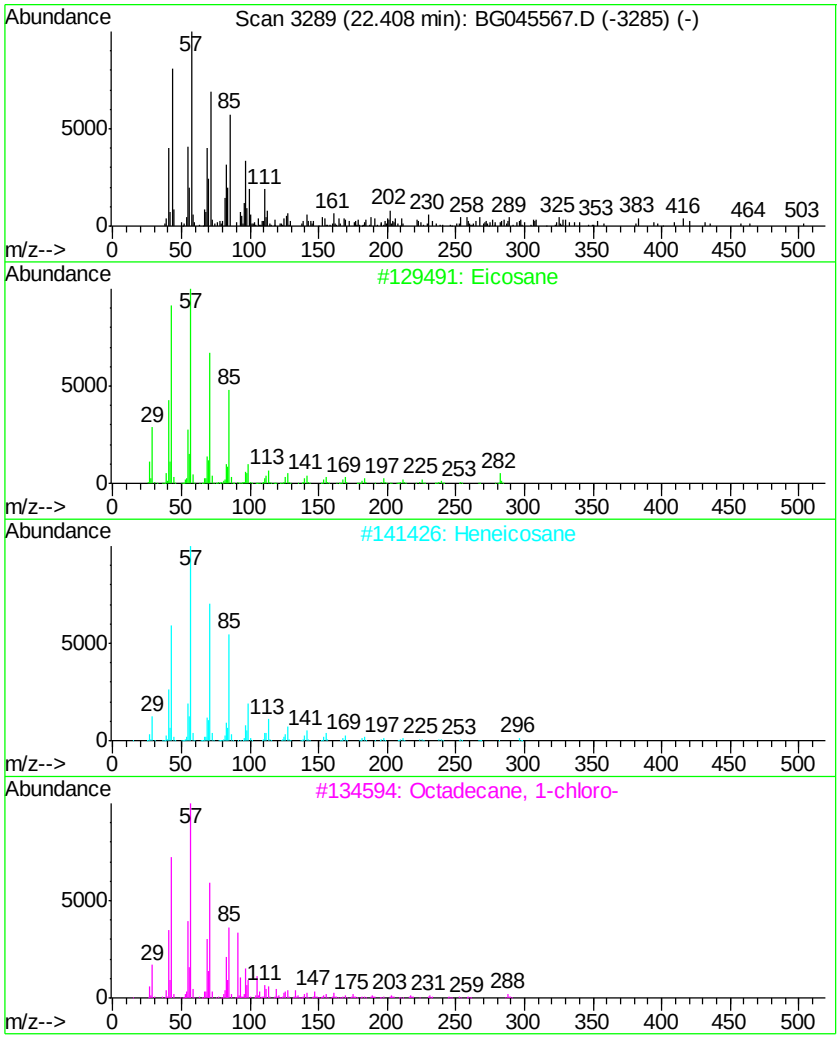
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

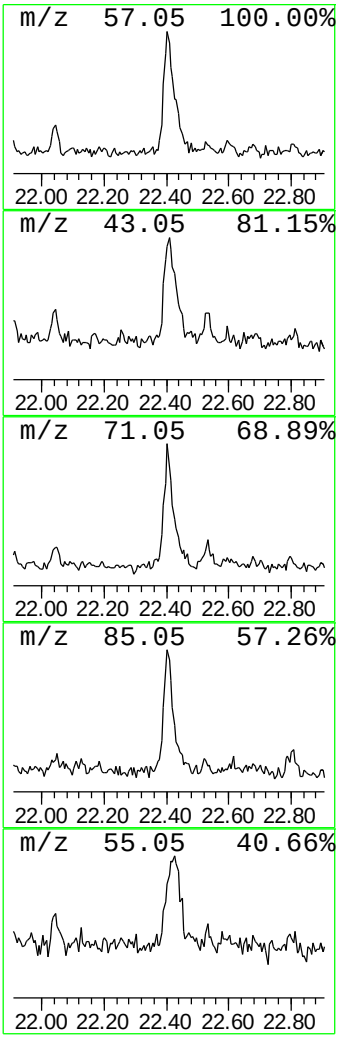
****

Peak Number 5 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	4.39 ng	280772	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	64
2	Heneicosane	296	C21H44	000629-94-7	64
3	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	62
4	Hexadecane	226	C16H34	000544-76-3	60
5	Tridecane	184	C13H28	000629-50-5	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

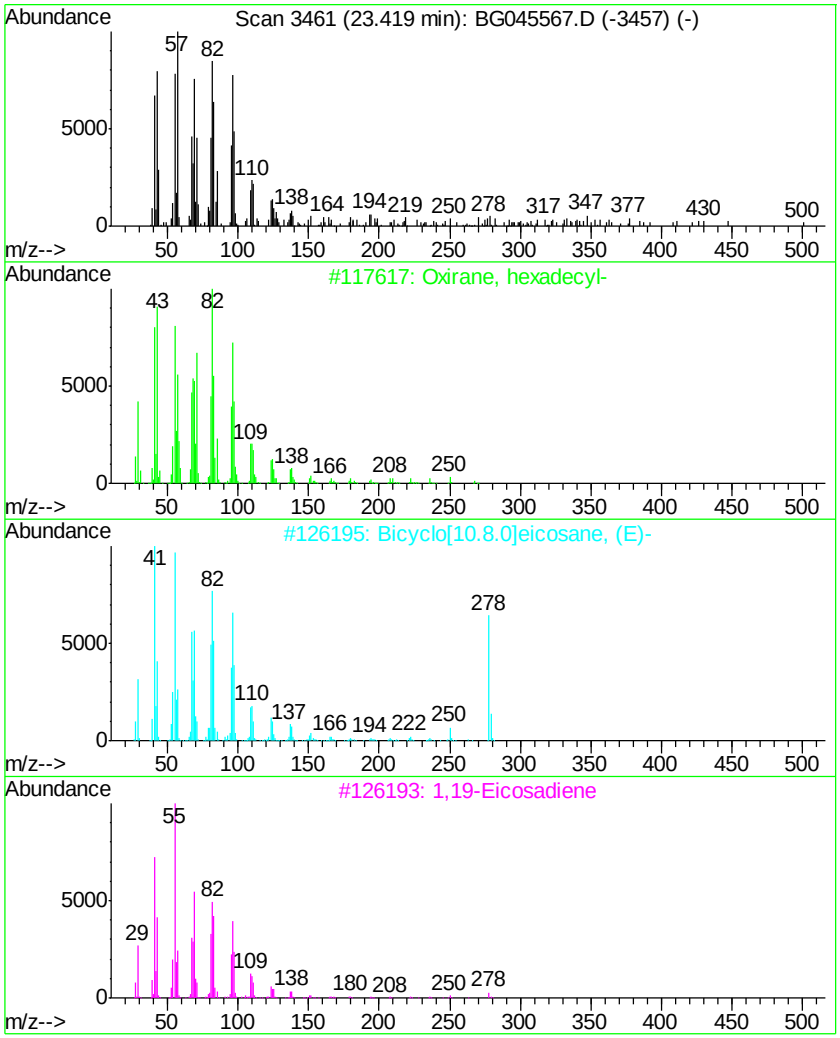
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

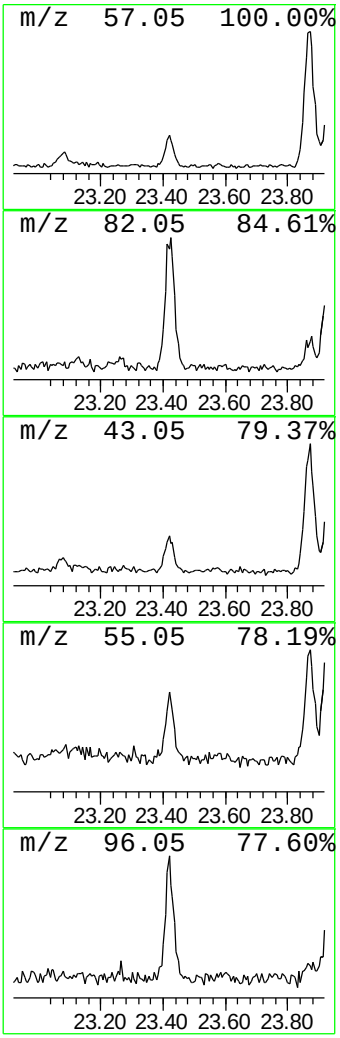
****

Peak Number 6 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.42	4.68 ng	255632	Perylene-d12	24.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2	Bicyclo[10.8.0]eicosane, (E)-	278	C20H38	1000155-85-0	93
3	1,19-Eicosadiene	278	C20H38	014811-95-1	93
4	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	90
5	17-Octadecenal	266	C18H34O	056554-86-0	78





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

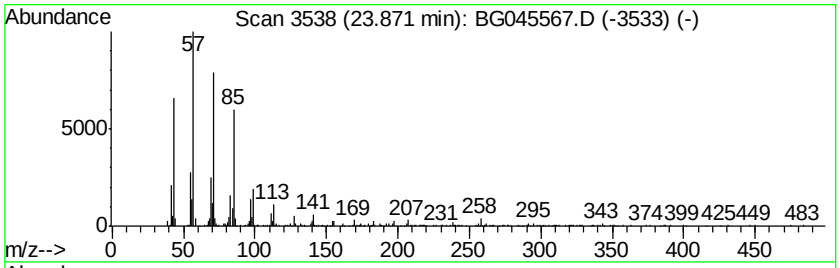
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

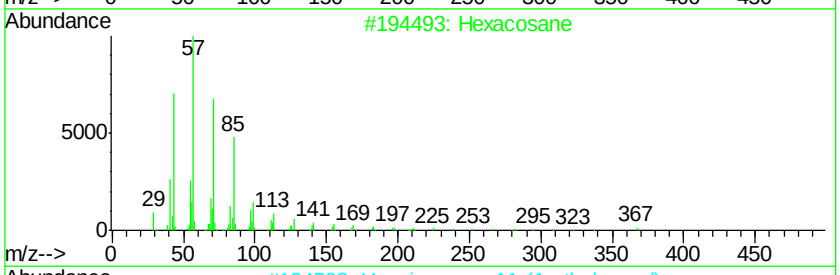
****

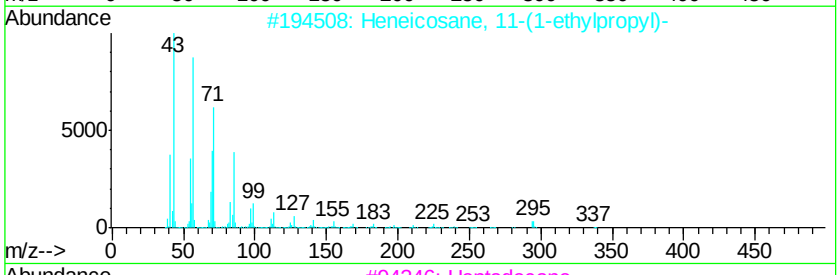
Peak Number 7 Hexacosane Concentration Rank 4

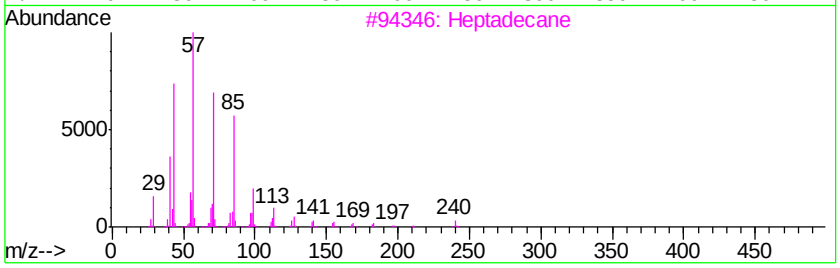
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.87	7.11 ng	388537	Perylene-d12	24.76

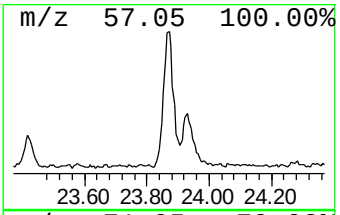
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3	Heptadecane	240	C17H36	000629-78-7	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	86

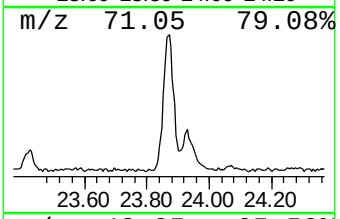


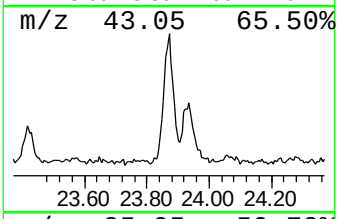


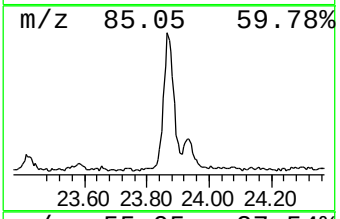


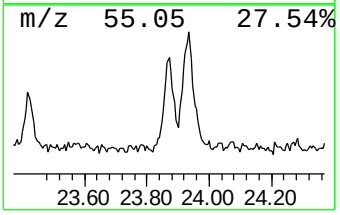












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

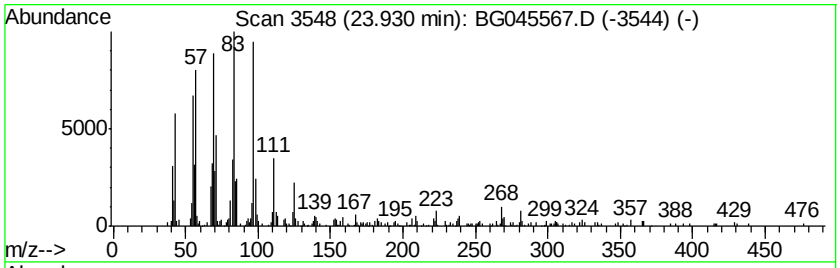
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

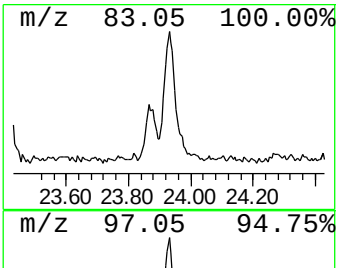
****

Peak Number 8 1-Heptadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	6.70 ng	366410	Perylene-d12	24.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	90
2	3-Heptadecene, (Z)-	238	C17H34	1000141-67-3	83
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	70
4	E-14-Hexadecenal	238	C16H30O	330207-53-9	64
5	2-Methyl-2-docosene	322	C23H46	1000131-16-9	55





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

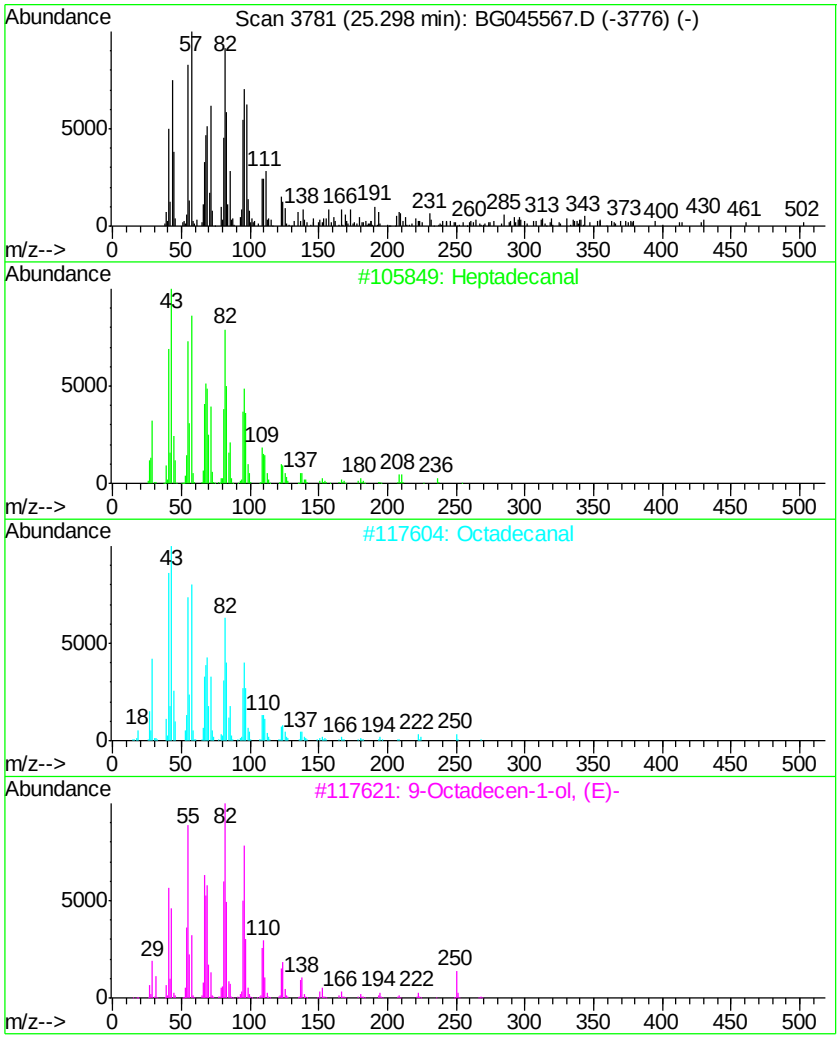
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

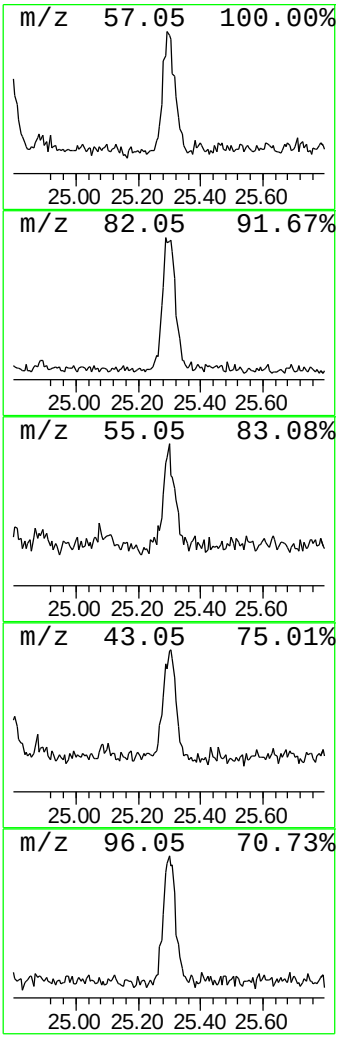
****

Peak Number 9 Heptadecanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.30	6.33 ng	346278	Perylene-d12	24.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanal	254	C17H34O	1000376-70-0	91
2	Octadecanal	268	C18H36O	000638-66-4	91
3	9-Octadecen-1-ol, (E)-	268	C18H36O	000506-42-3	90
4	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	90
5	1,21-Docosadiene	306	C22H42	053057-53-7	89





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

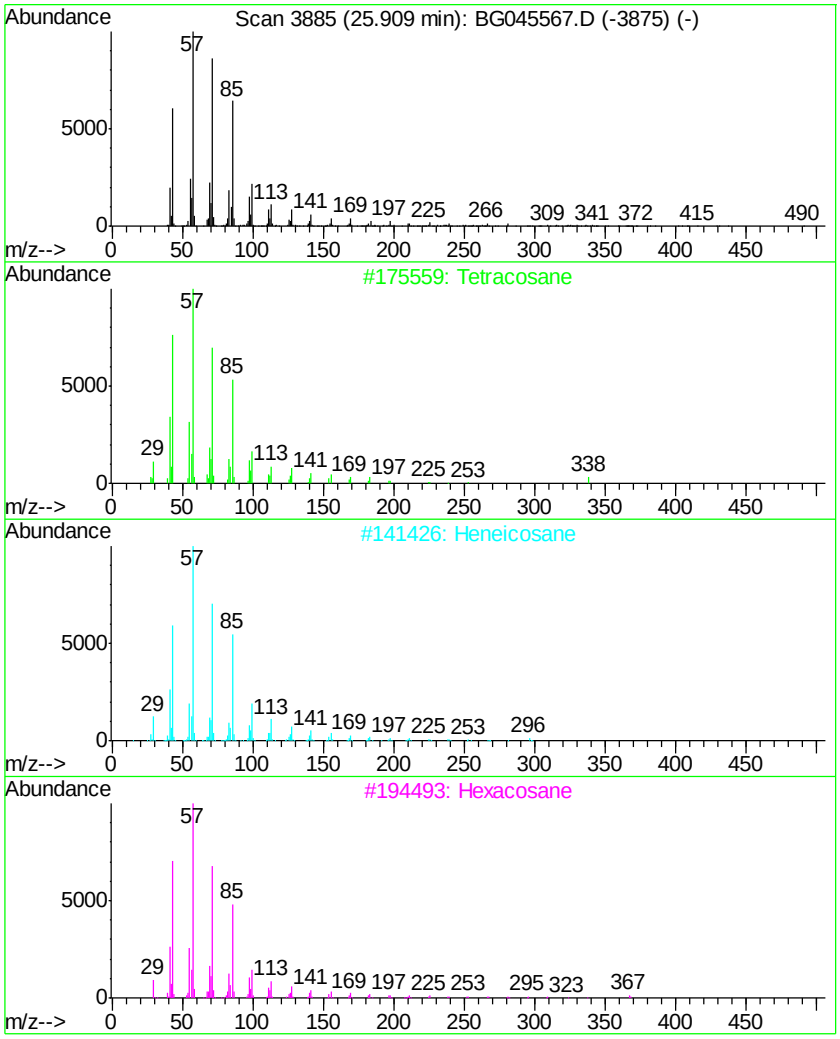
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

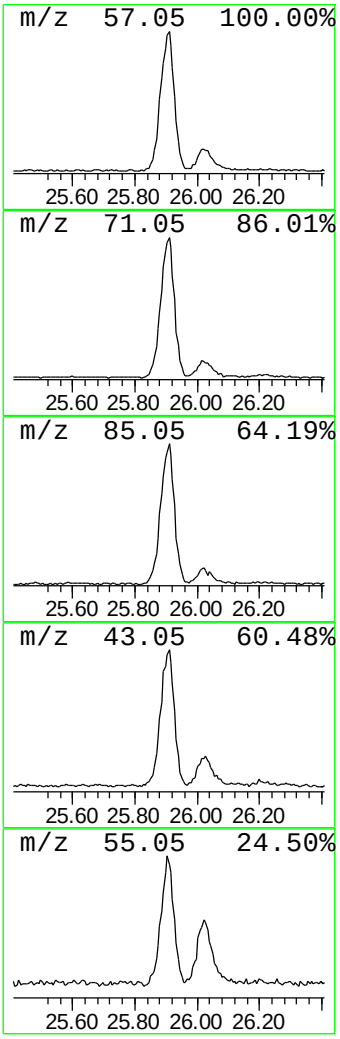
****

Peak Number 10 Tetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.91	32.76 ng	1791020	Perylene-d12	24.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	2-methyltetracosane	352	C25H52	1000376-72-6	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

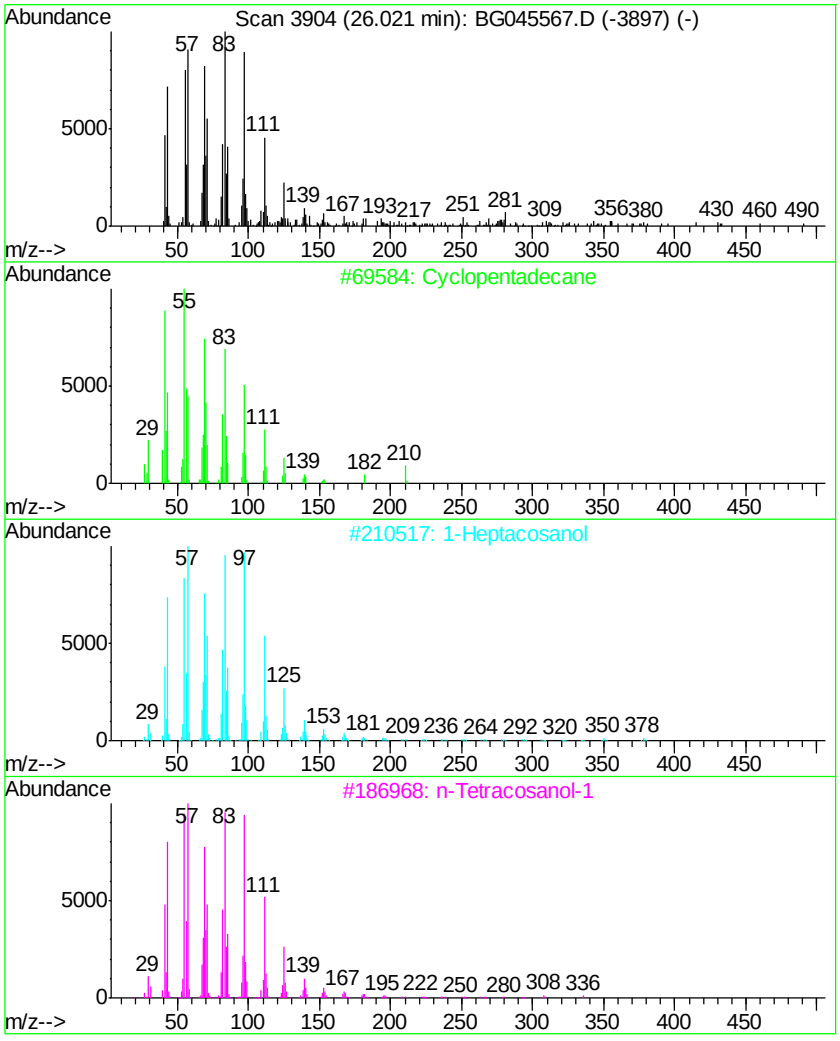
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

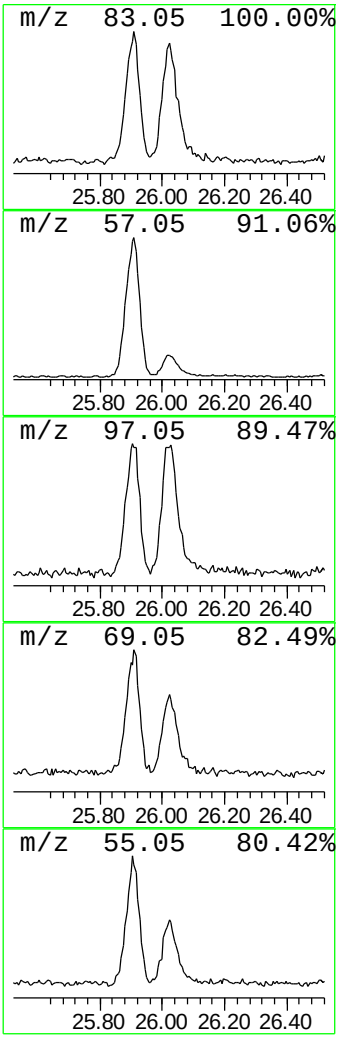
****

Peak Number 11 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.02	10.49 ng	573624	Perylene-d12	24.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG060120\
Data File : BG045567.D
Acq On : 1 Jun 2020 22:37
Operator : CG/JU
Sample : L2792-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM97-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.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
unknown18.26	18.26	2.5	ng	134569	4	17.34	1079750	20.0
unknown19.34	19.34	3.5	ng	189177	4	17.34	1079750	20.0
Dichloroacetic ac...	21.26	5.3	ng	339232	5	21.60	1278890	20.0
Eicosane	22.41	4.4	ng	280772	5	21.60	1278890	20.0
Oxirane, hexadecyl-	23.42	4.7	ng	255632	6	24.76	1093560	20.0
Hexacosane	23.87	7.1	ng	388537	6	24.76	1093560	20.0
1-Heptadecene	23.93	6.7	ng	366410	6	24.76	1093560	20.0
Heptadecanal	25.30	6.3	ng	346278	6	24.76	1093560	20.0
Tetracosane	25.91	32.8	ng	1791020	6	24.76	1093560	20.0
Cyclopentadecane	26.02	10.5	ng	573624	6	24.76	1093560	20.0