LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050919\
Data File : BG040838.D
Acq On : 10 May 2019 6:30
Operator : HP/JU
Sample : K2764-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-0612-01

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-BG042319.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	3.153	6	11	20	rBV	119820	216119	4.97%	0.830%
2	3.229	20	24	34	rVB	248767	333019	7.66%	1.279%
3	5.673	433	440	454	rVB	1120716	1763737	40.55%	6.775%
4	7.277	704	713	723	rBV	1215319	2127343	48.91%	8.172%
5	7.665	771	779	789	rBV	1158266	1956023	44.97%	7.514%
6	8.141	852	860	871	rBV	209011	352829	8.11%	1.355%
7	8.464	906	915	922	rBV	786387	1345172	30.93%	5.167%
8	9.316	1052	1060	1068	rBV	732964	1329142	30.56%	5.106%
9	10.961	1332	1340	1348	rBV	270965	496434	11.41%	1.907%
10	13.394	1745	1754	1764	rBV	1798224	2725454	62.66%	10.469%
11	14.210	1887	1893	1899	rBV	327013	457222	10.51%	1.756%
12	14.769	1980	1988	1997	rBV2	494129	780583	17.95%	2.999%
13	16.255	2234	2241	2254	rBV	1799341	2777007	63.85%	10.668%
14	17.512	2449	2455	2462	rBV2	714126	1060286	24.38%	4.073%
15	18.364	2594	2600	2614	rBV2	285263	432226	9.94%	1.660%
16	19.628	2810	2815	2823	rBV2	93162	146513	3.37%	0.563%
17	20.109	2890	2897	2906	rBV	3287592	4349288	100.00%	16.707%
18	21.396	3110	3116	3131	rBV2	179497	454258	10.44%	1.745%
19	21.796	3177	3184	3197	rVB2	686645	1131499	26.02%	4.347%
20	21.948	3206	3210	3216	rVB2	28664	48096	1.11%	0.185%
21	22.577	3312	3317	3322	rBV2	47387	74065	1.70%	0.285%
22	23.294	3431	3439	3447	rBV2	75437	164179	3.77%	0.631%
23	23.494	3468	3473	3480	rVB3	47041	90403	2.08%	0.347%
24	24.128	3574	3581	3590	rVB2	64091	128075	2.94%	0.492%
25	25.150	3737	3755	3770	rBV2	317151	1168813	26.87%	4.490%
26	26.296	3939	3950	3961	rBV6	37487	124541	2.86%	0.478%

Sum of corrected areas: 26032326

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Misc :
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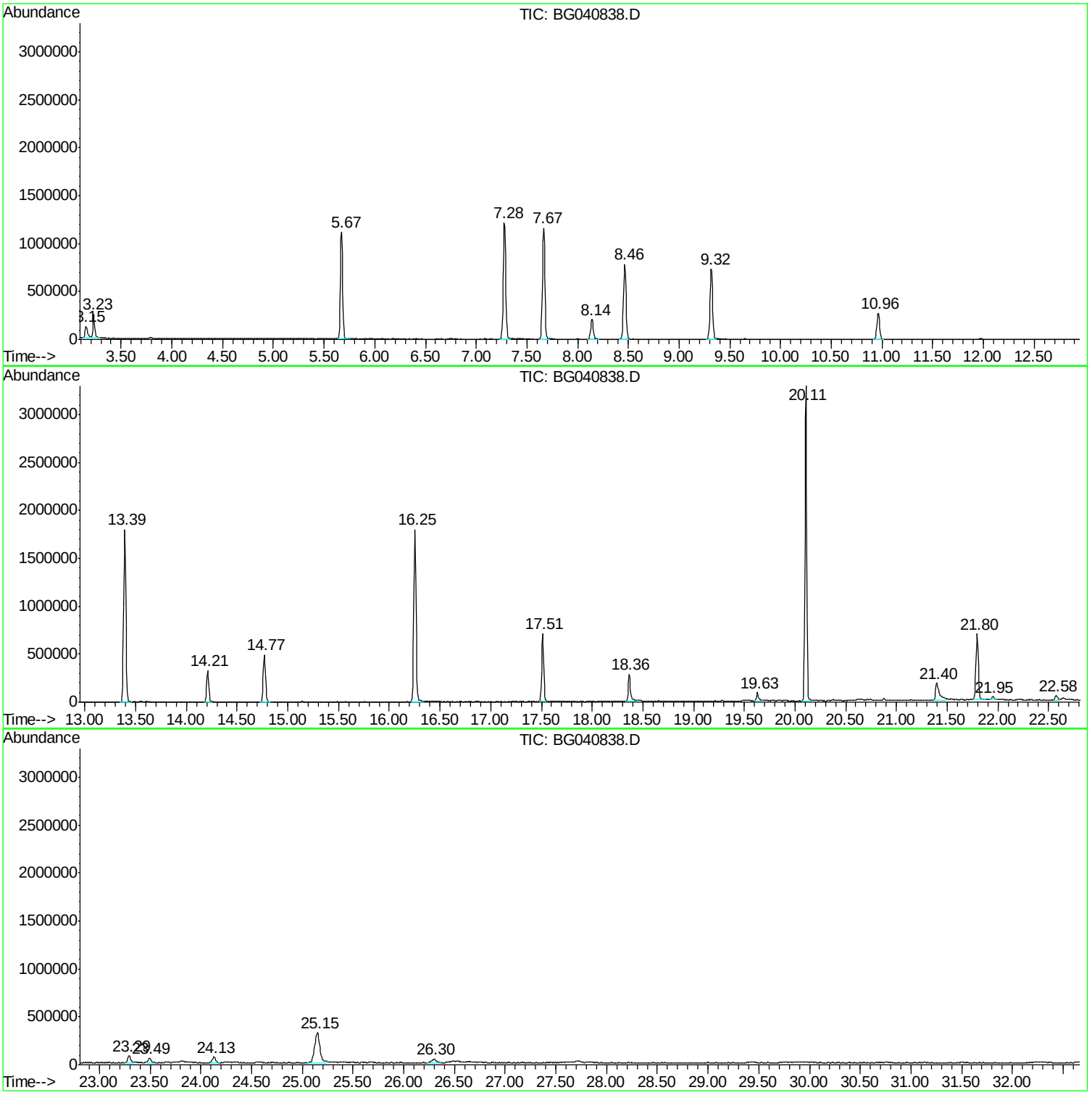
Instrument :
BNA_G
ClientSampleId :
P021-SS008-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BG040838.D
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Misc :
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Instrument : BNA_G
ClientSampleId : P021-SS008-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

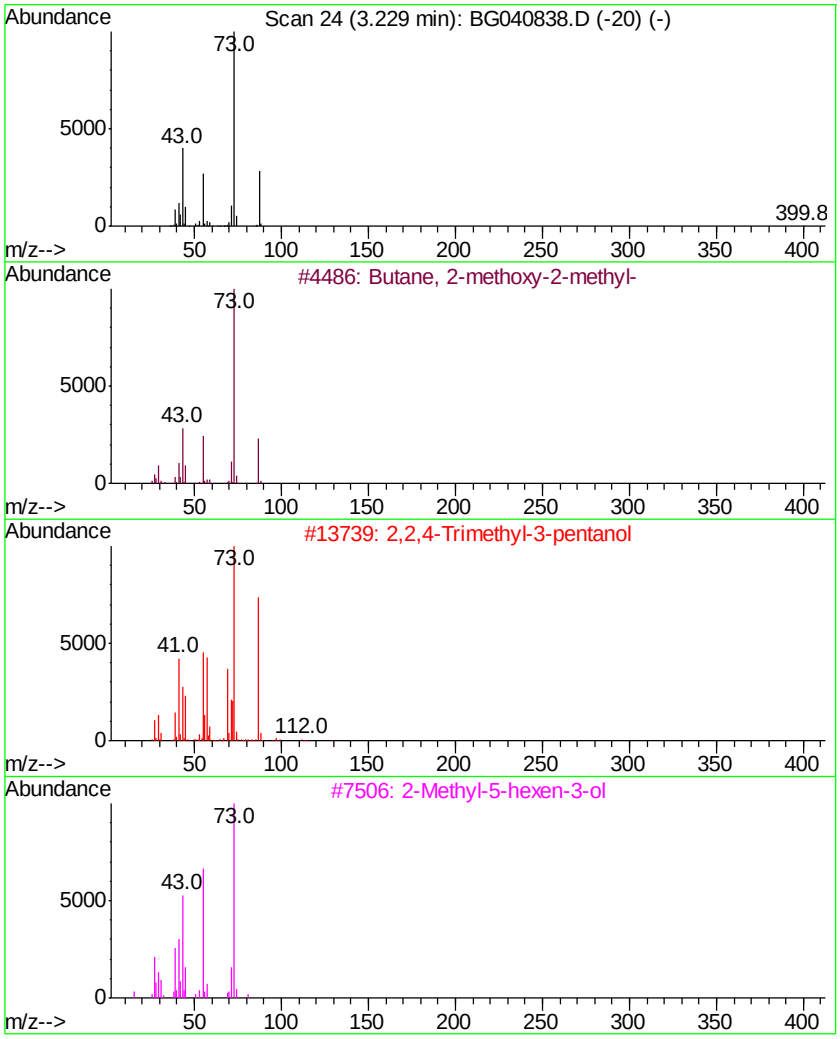
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

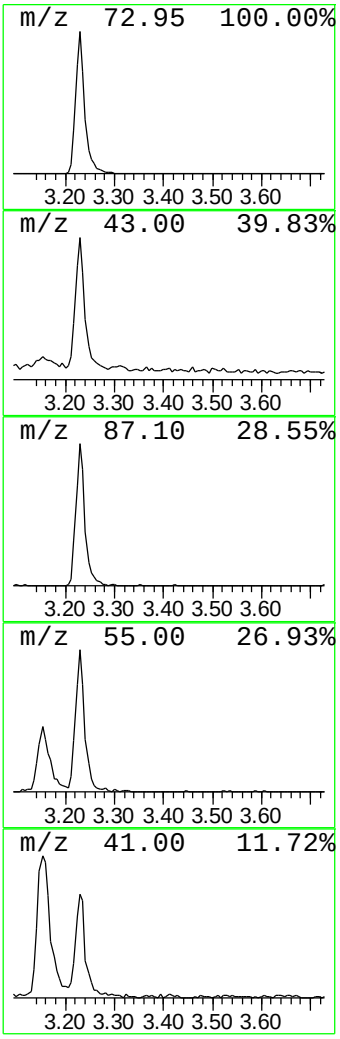
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	18.88 ng	333019	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	25





Library Search Compound Report

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Operator : HP/JU
Sample : K2764-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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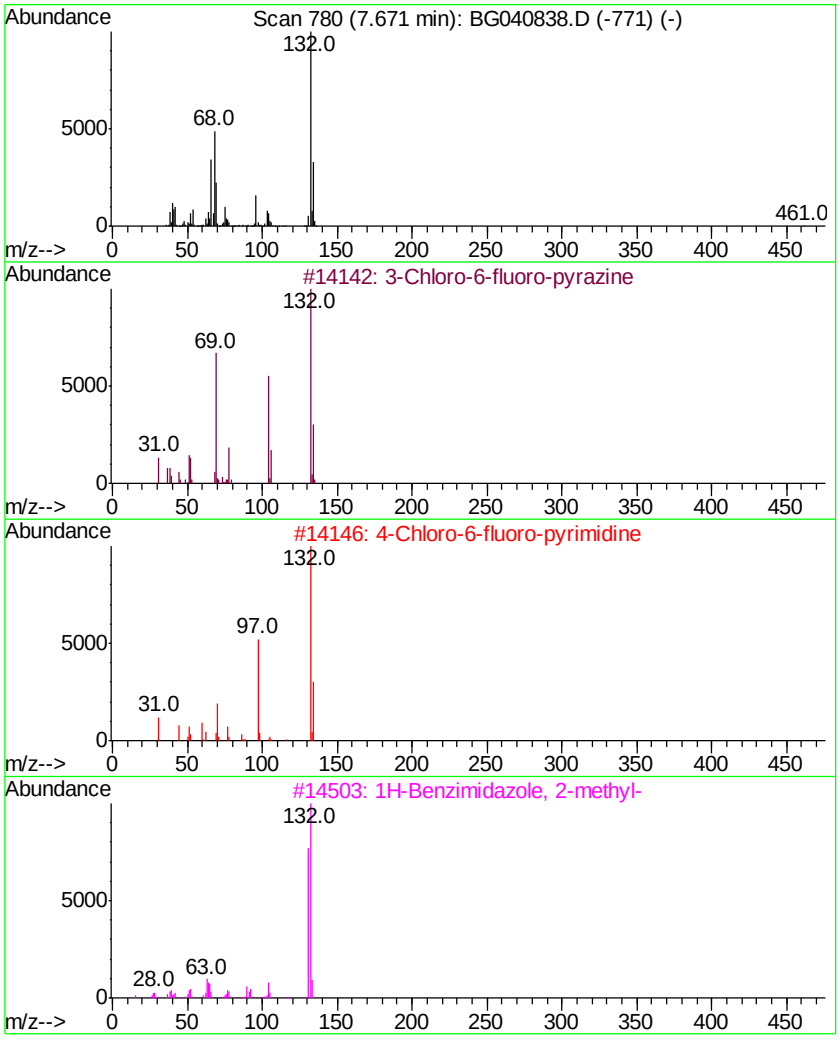
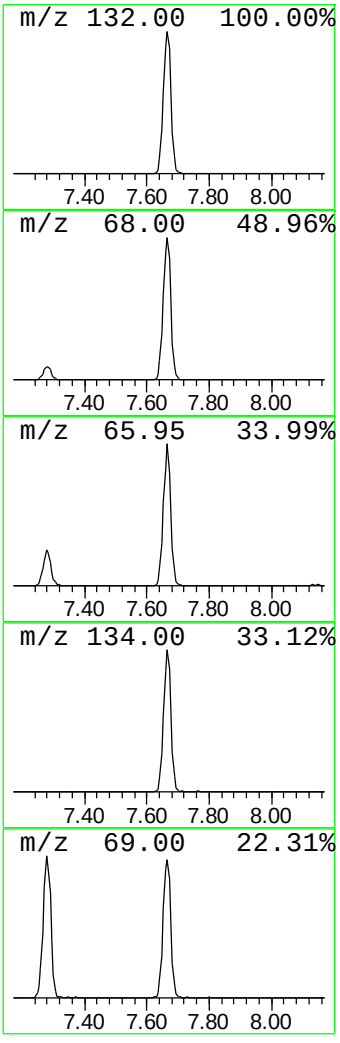
Peak Number 3 unknown7.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	110.88 ng	1956020	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12





Library Search Compound Report

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Data File : BG040838.D
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Operator : HP/JU
Sample : K2764-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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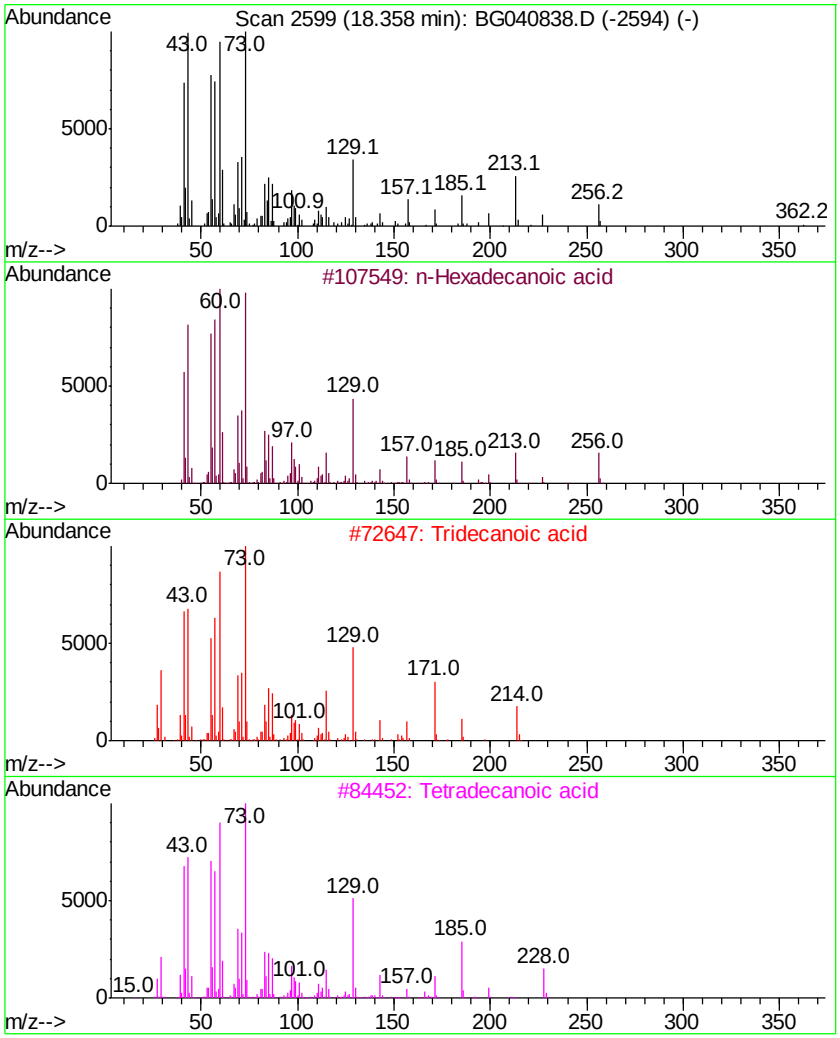
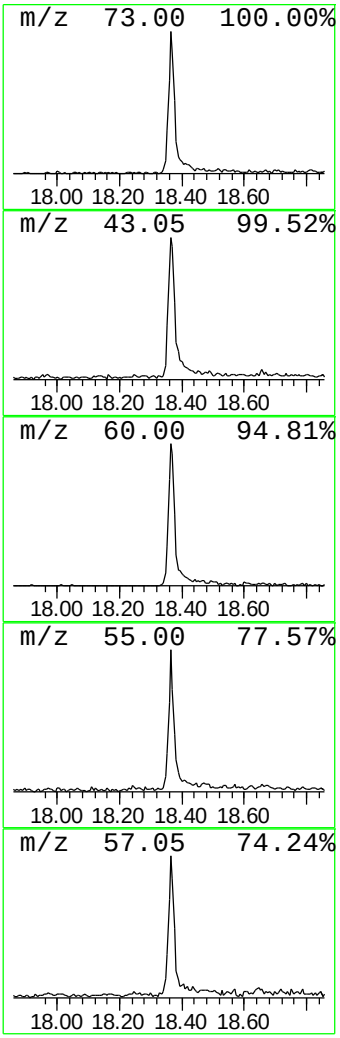
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	8.15 ng	432226	Phenanthrene-d10	17.51

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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





Library Search Compound Report

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Operator : HP/JU
Sample : K2764-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

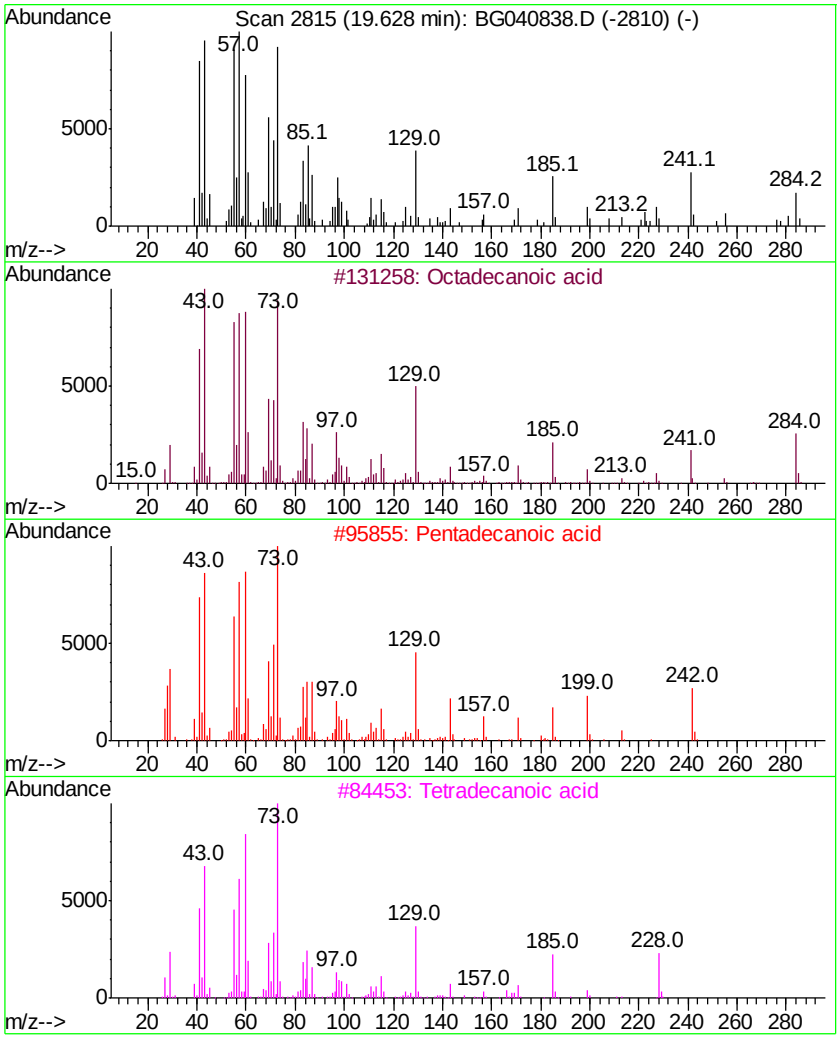
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

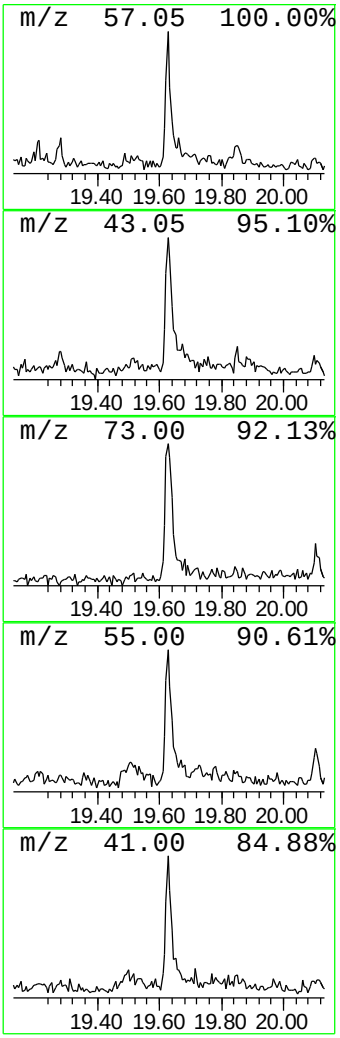
****

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.63	2.76 ng	146513	Phenanthrene-d10	17.51

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	45
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	30





Library Search Compound Report

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Operator : HP/JU
Sample : K2764-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P021-SS008-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

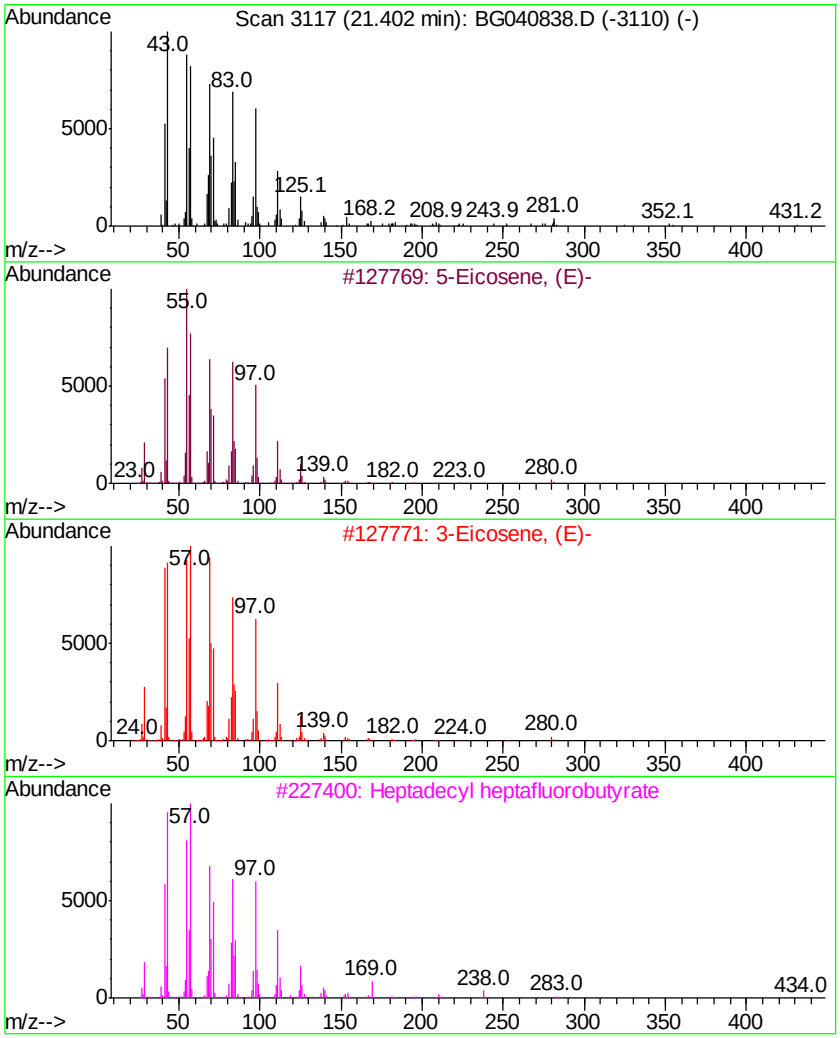
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

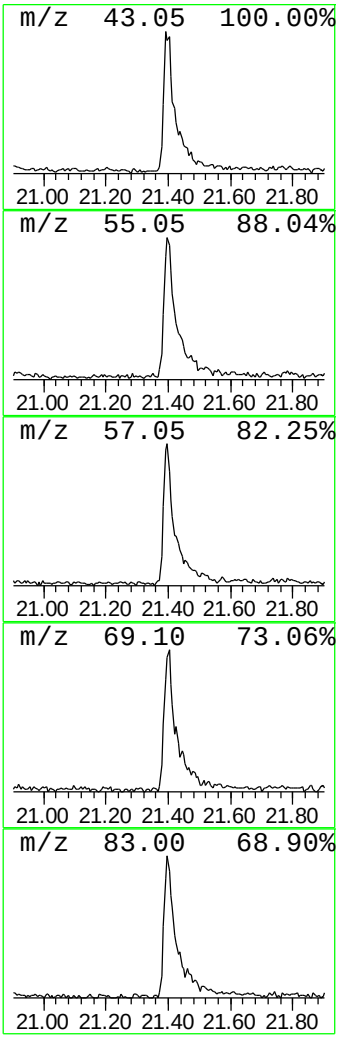
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	8.03 ng	454258	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91





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Instrument : BNA_G
ClientSampleId : P021-SS008-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

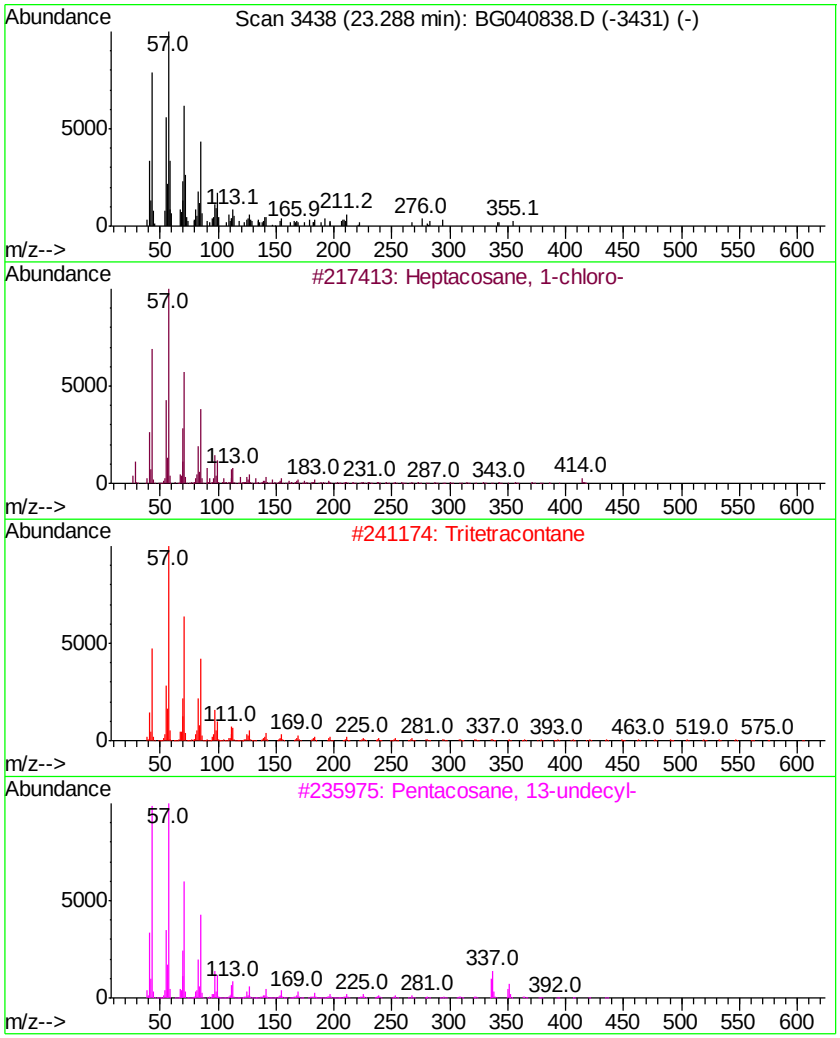
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

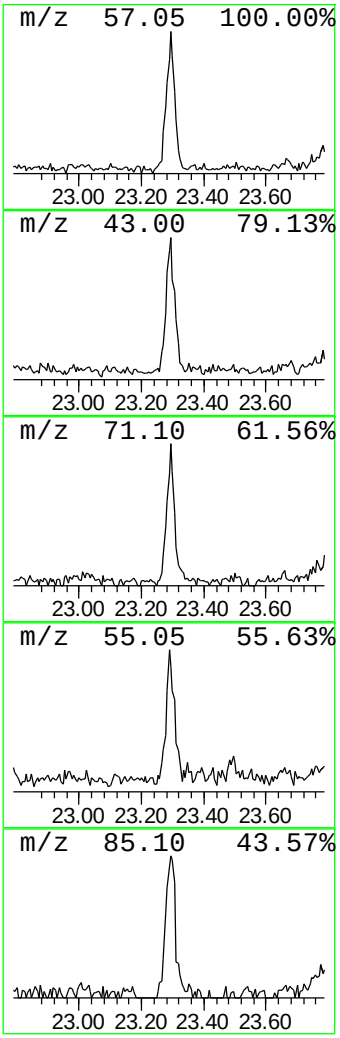
****

Peak Number 8 Heptacosane, 1-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.29	2.90 ng	164179	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	70
2	Tritetracontane	605	C43H88	007098-21-7	62
3	Pentacosane, 13-undecyl-	507	C36H74	055517-89-0	58
4	Octacosane	394	C28H58	000630-02-4	58
5	Heptacosane	380	C27H56	000593-49-7	58





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Misc :
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Instrument : BNA_G
ClientSampleId : P021-SS008-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

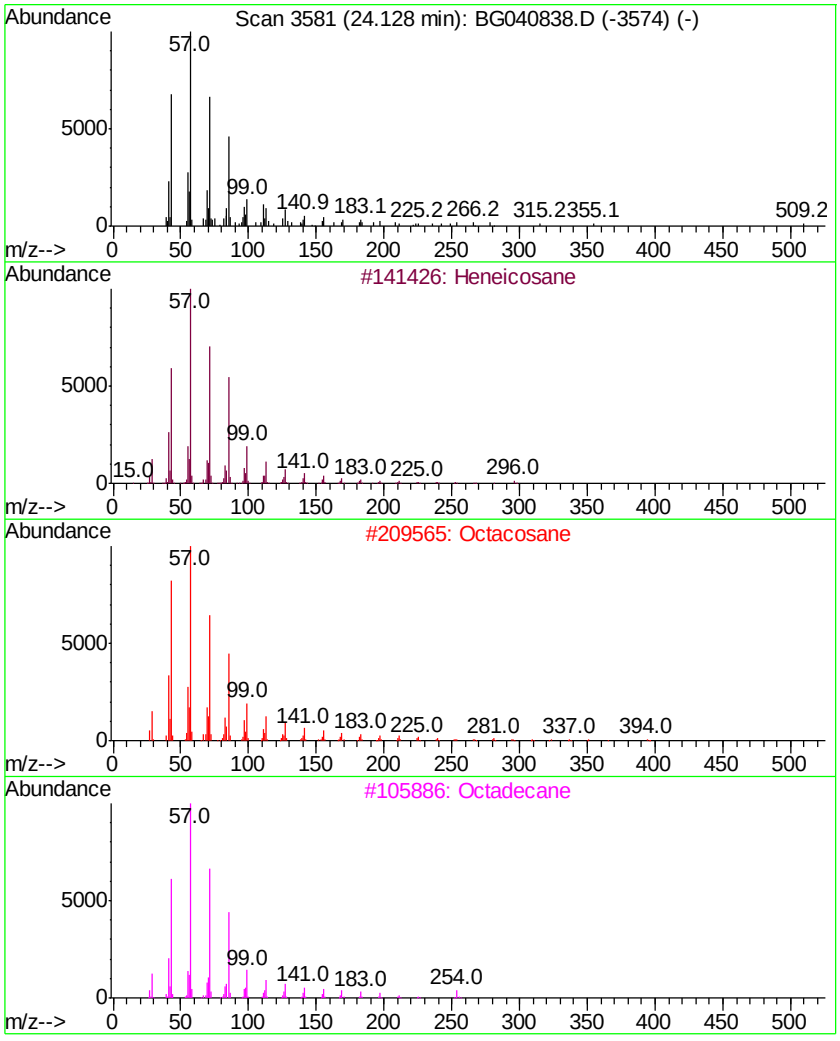
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

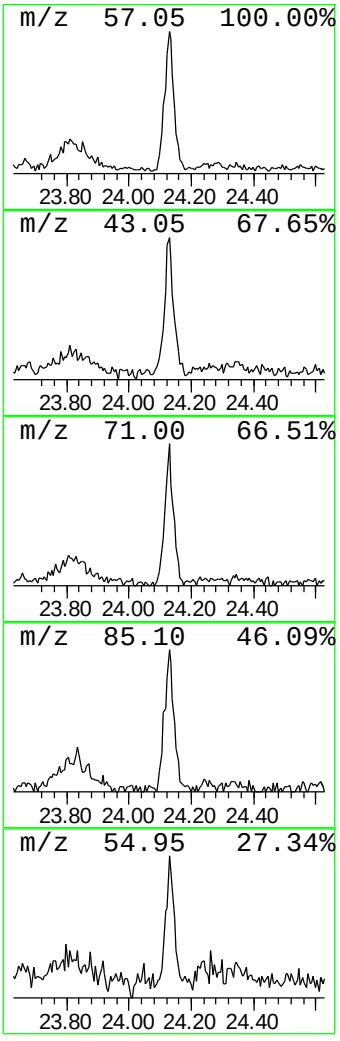
****

Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.13	2.19 ng	128075	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Octadecane	254	C18H38	000593-45-3	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





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Misc :
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Instrument : BNA_G
ClientSampleId : P021-SS008-0612-01

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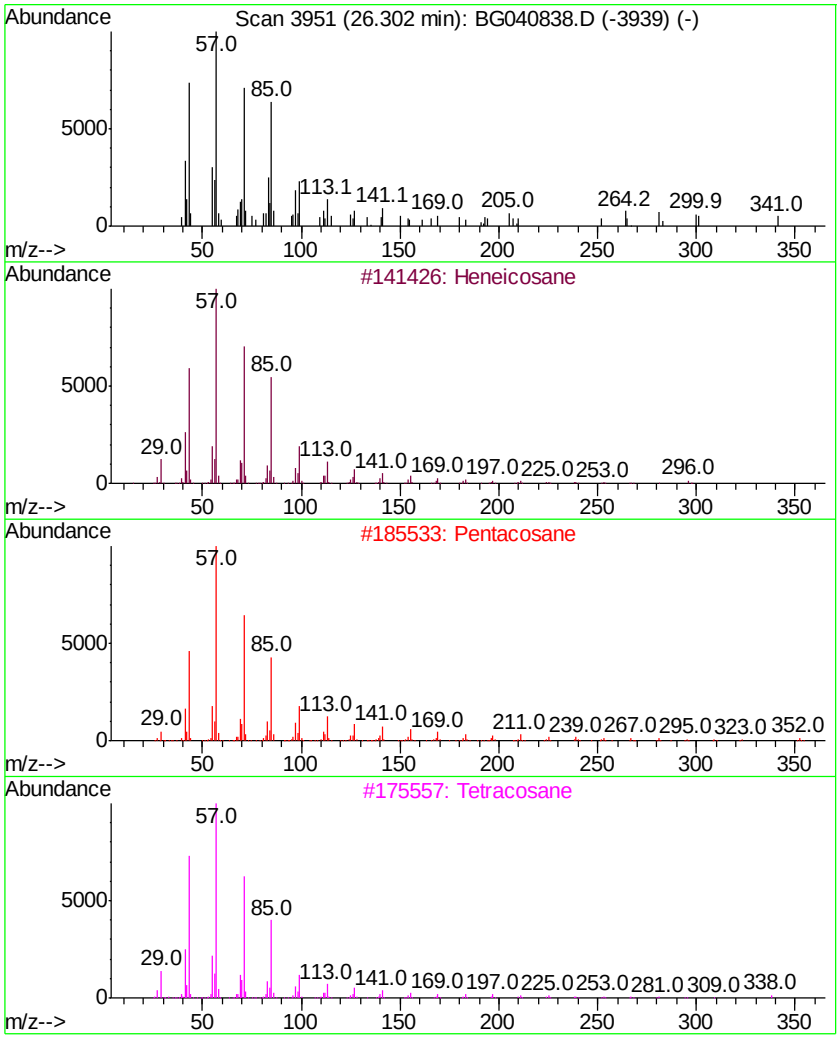
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

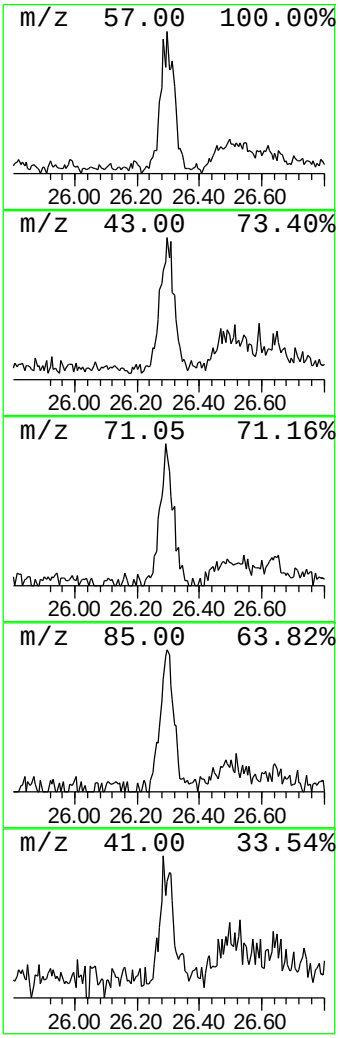
****

Peak Number 10 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.30	2.13 ng	124541	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	74
2	Pentacosane	352	C25H52	000629-99-2	72
3	Tetracosane	338	C24H50	000646-31-1	72
4	2-methyloctacosane	408	C29H60	1000376-72-8	72
5	Nonadecane	268	C19H40	000629-92-5	72





Tentatively Identified Compound (LSC) summary

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Misc :
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ClientSampleId : P021-SS008-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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
Butane, 2-methoxy...	3.23	18.9	ng	333019	1	8.14	352829	20.0
unknown7.67	7.67	110.9	ng	1956020	1	8.14	352829	20.0
n-Hexadecanoic acid	18.36	8.2	ng	432226	4	17.51	1060290	20.0
Octadecanoic acid	19.63	2.8	ng	146513	4	17.51	1060290	20.0
5-Eicosene, (E)-	21.40	8.0	ng	454258	5	21.80	1131500	20.0
Heptacosane, 1-ch...	23.29	2.9	ng	164179	5	21.80	1131500	20.0
Heneicosane	24.13	2.2	ng	128075	6	25.15	1168810	20.0
Pentacosane	26.30	2.1	ng	124541	6	25.15	1168810	20.0