LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040965.D
Acq On : 31 May 2019 00:38
Operator : HP/JU
Sample : K3090-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4-S

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-BG052919.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	3.129	3	7	16	rVV	117725	224640	4.51%	0.828%
2	3.206	16	20	31	rVB	340538	503080	10.11%	1.853%
3	5.656	429	437	448	rBV	1065285	1677516	33.70%	6.180%
4	7.266	702	711	730	rBV	1162131	1974132	39.66%	7.272%
5	7.648	768	776	786	rBV	1089590	1832195	36.81%	6.749%
6	8.123	850	857	867	rVB	242095	410728	8.25%	1.513%
7	8.447	904	912	923	rBV	795832	1354932	27.22%	4.991%
8	9.299	1048	1057	1069	rBV	687130	1230361	24.72%	4.532%
9	10.944	1330	1337	1345	rVB	321356	560364	11.26%	2.064%
10	13.376	1742	1751	1760	rBV	1942000	2964205	59.55%	10.919%
11	14.193	1881	1890	1896	rBV	209083	313642	6.30%	1.155%
12	14.751	1975	1985	1994	rBV2	532217	863095	17.34%	3.179%
13	16.238	2231	2238	2251	rBV	1793289	2661625	53.47%	9.805%
14	17.495	2445	2452	2462	rBV2	780326	1205660	24.22%	4.441%
15	18.347	2592	2597	2607	rBV	235385	350596	7.04%	1.292%
16	19.610	2808	2812	2818	rBV2	97257	139603	2.80%	0.514%
17	20.092	2886	2894	2904	rBV	3742347	4977574	100.00%	18.336%
18	21.367	3106	3111	3121	rBV	189154	326505	6.56%	1.203%
19	21.772	3173	3180	3190	rBV2	821456	1427704	28.68%	5.259%
20	21.925	3202	3206	3213	rVB3	62744	102182	2.05%	0.376%
21	22.548	3307	3312	3316	rBV3	63184	106249	2.13%	0.391%
22	23.259	3427	3433	3440	rBV2	80472	163228	3.28%	0.601%
23	24.087	3569	3574	3585	rVB4	77644	181453	3.65%	0.668%
24	25.115	3733	3749	3759	rBV2	434321	1457192	29.28%	5.368%
25	26.238	3934	3940	3949	rVB6	44215	137595	2.76%	0.507%

Sum of corrected areas: 27146056

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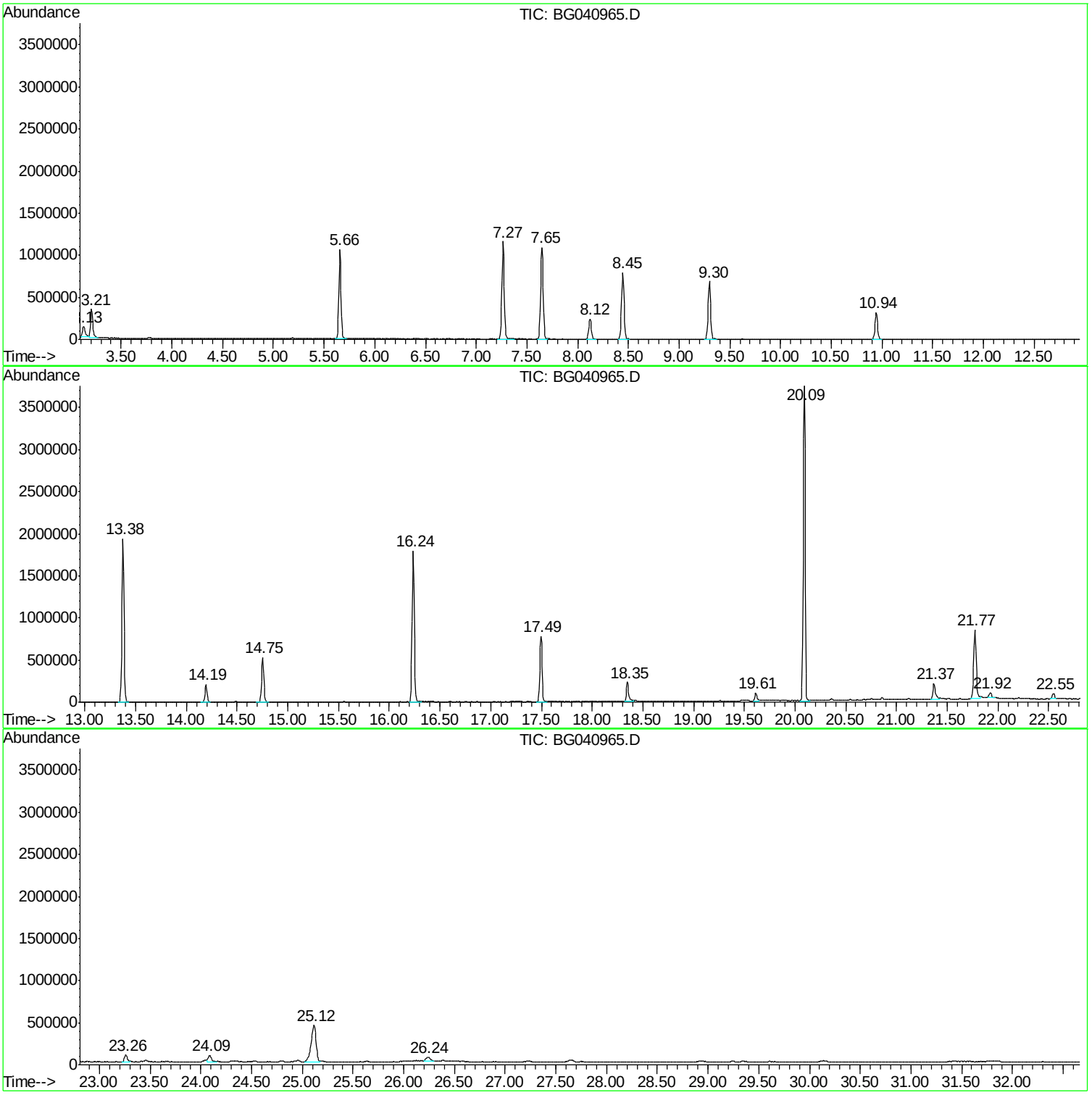
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040965.D
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Operator : HP/JU
Sample : K3090-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.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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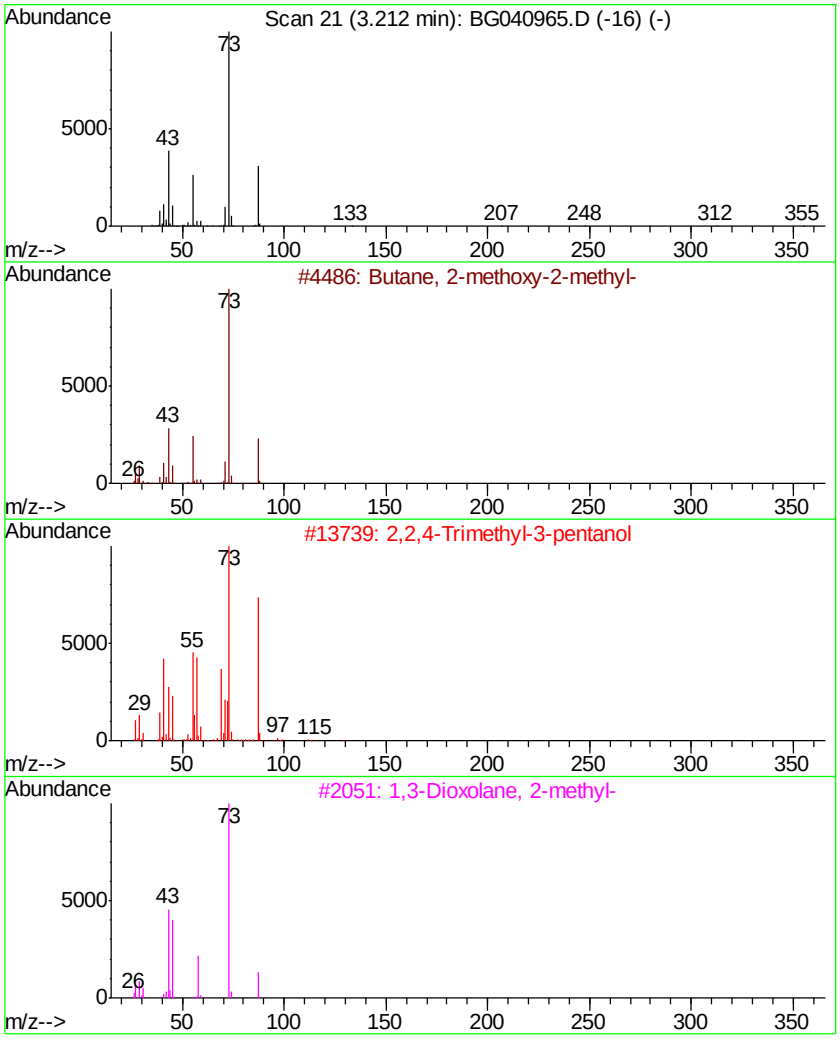
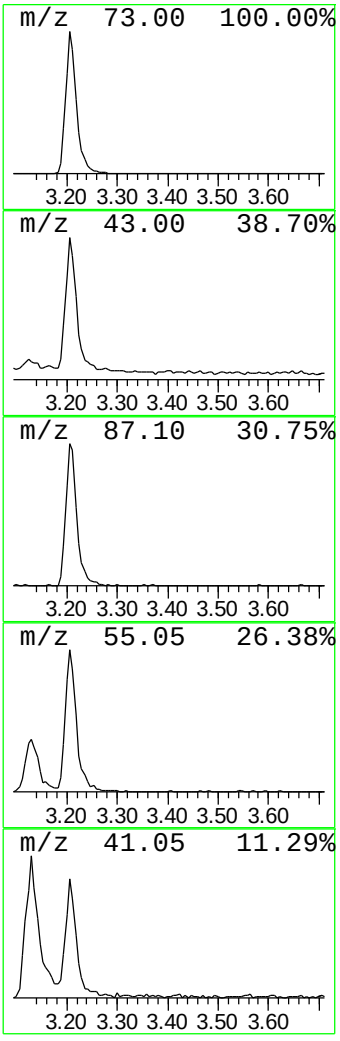
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	24.50 ng	503080	1,4-Dichlorobenzene-d4	8.12

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Library Search Compound Report

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Data File : BG040965.D
Acq On : 31 May 2019 00:38
Operator : HP/JU
Sample : K3090-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

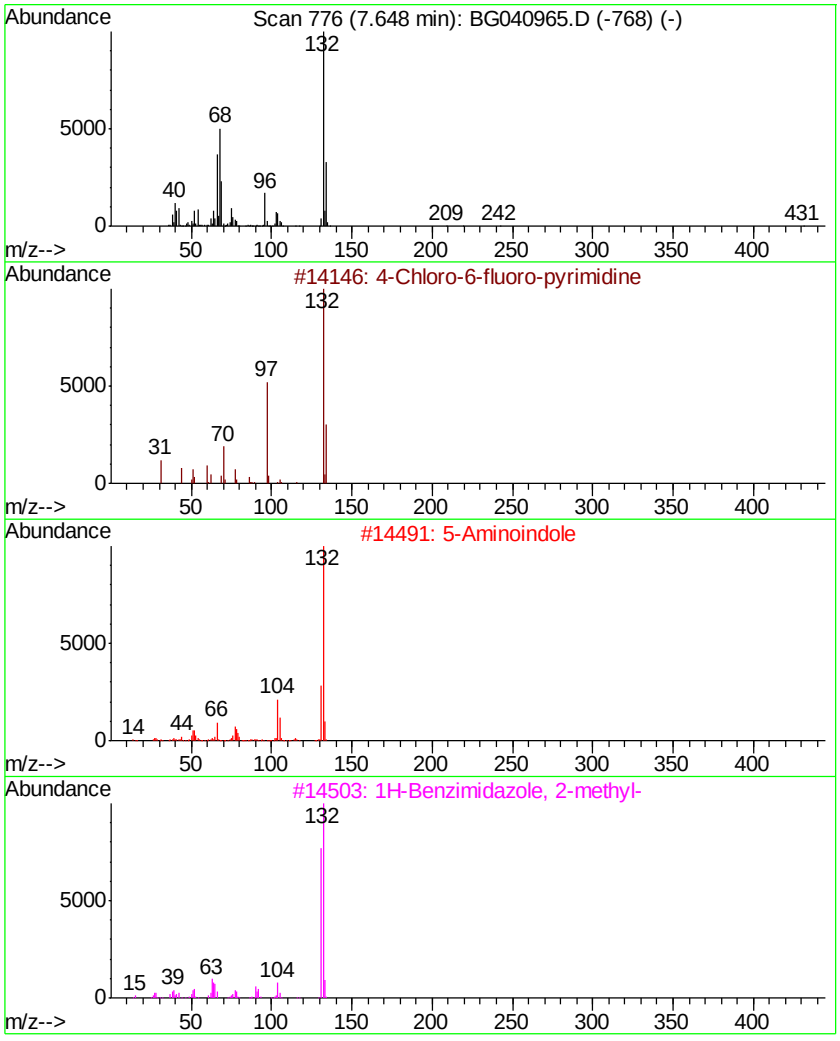
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

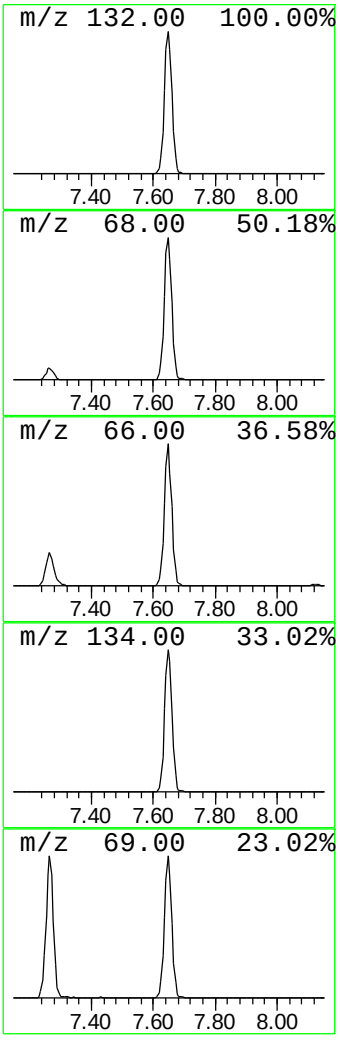
****

Peak Number 3 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	89.22 ng	1832200	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040965.D
Acq On : 31 May 2019 00:38
Operator : HP/JU
Sample : K3090-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

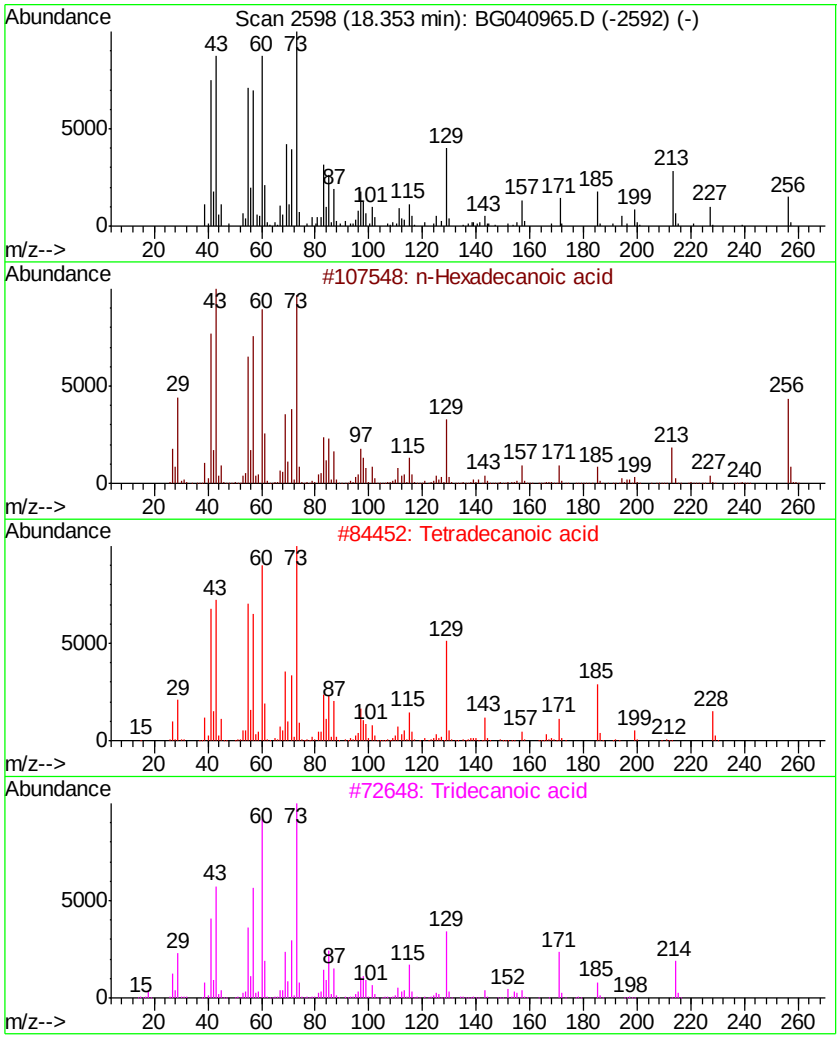
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

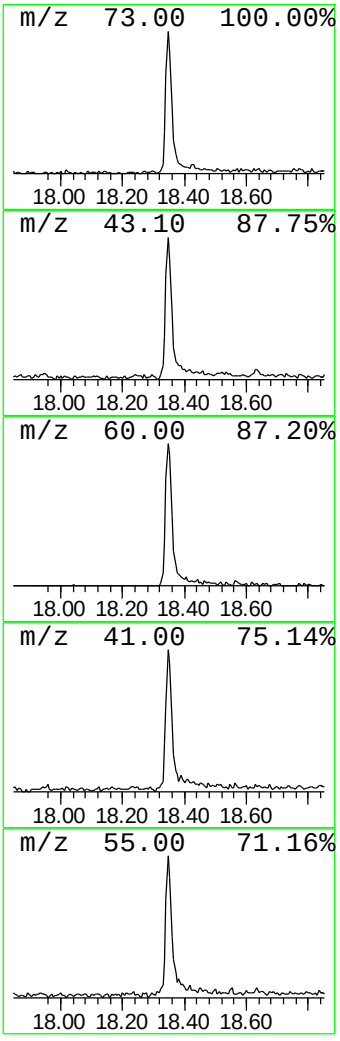
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	5.82 ng	350596	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040965.D
Acq On : 31 May 2019 00:38
Operator : HP/JU
Sample : K3090-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

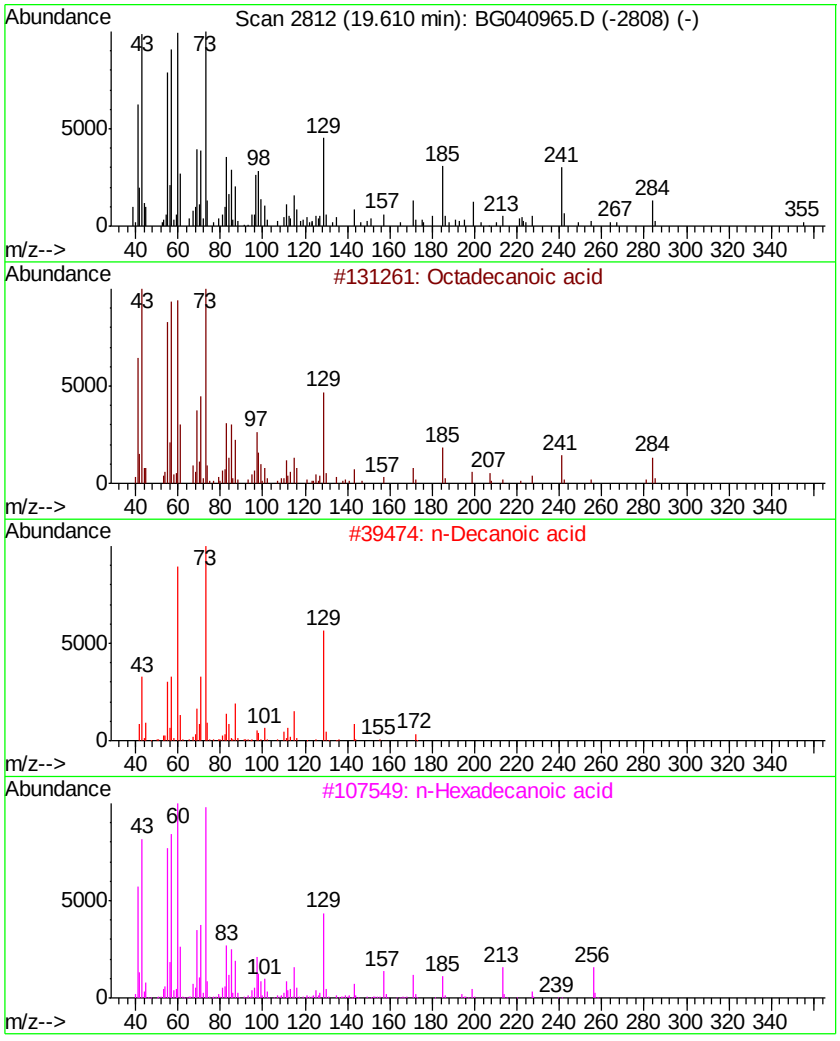
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

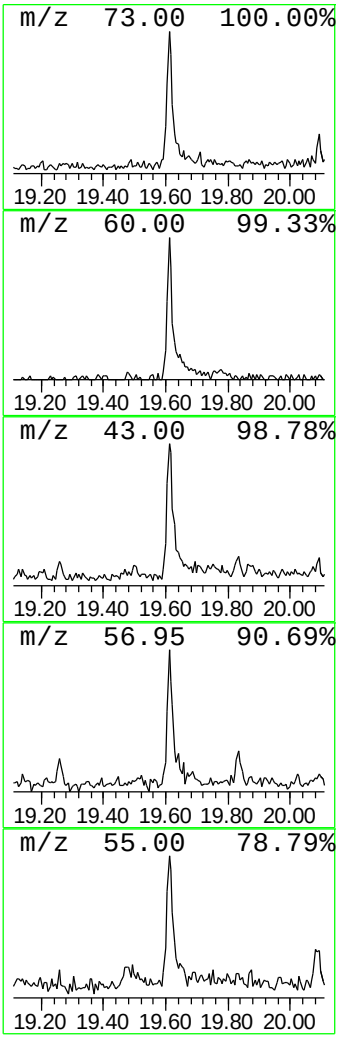
****

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	2.32 ng	139603	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	92
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
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Acq On : 31 May 2019 00:38
Operator : HP/JU
Sample : K3090-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
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TIC Library : C:\Database\NIST11.L
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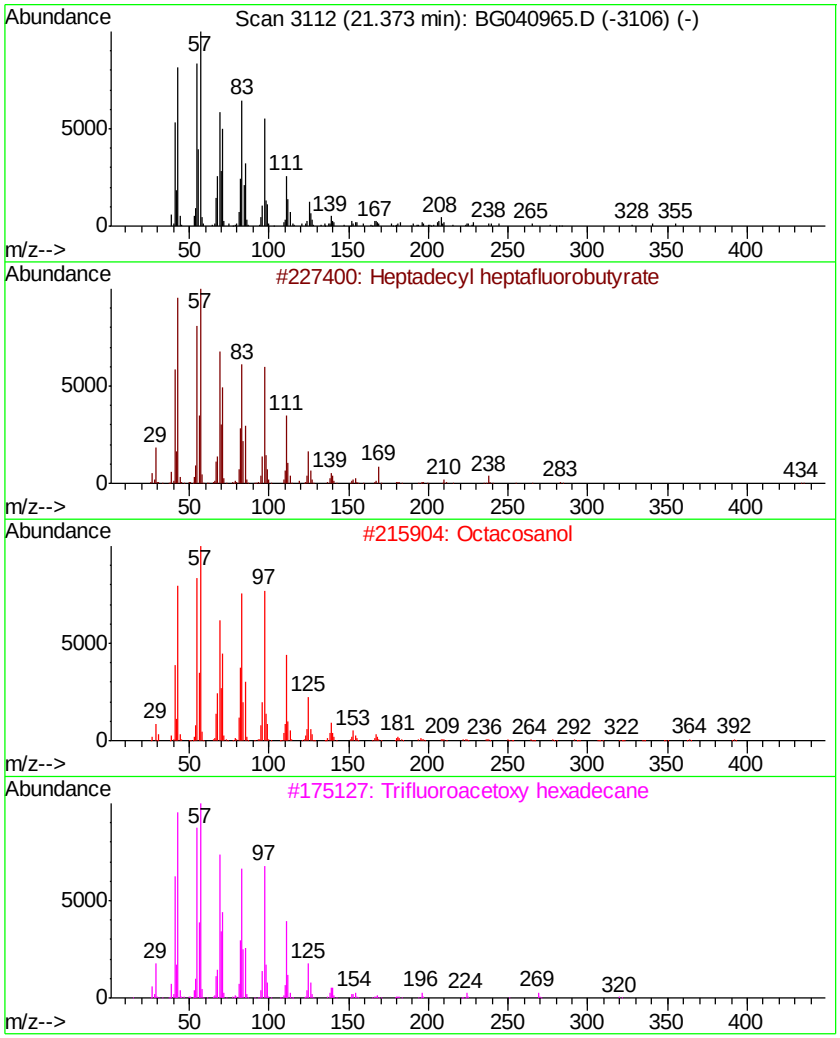
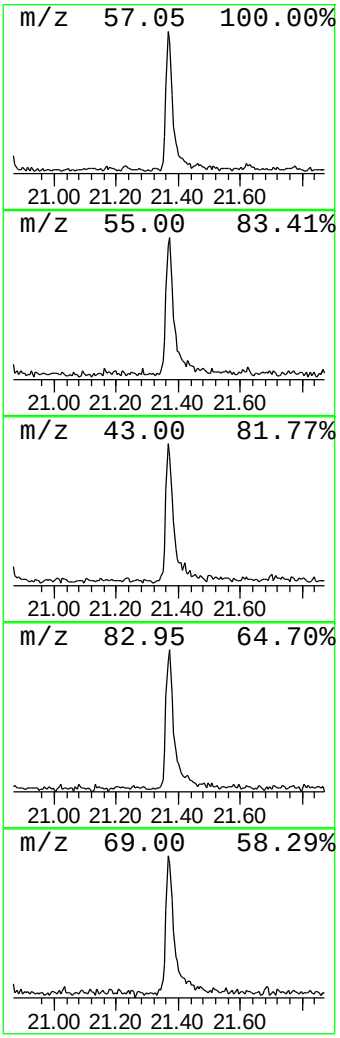
****

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	4.57 ng	326505	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Octacosanol	410	C28H58O	000557-61-9	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
4	1-Tricosene	322	C23H46	018835-32-0	87
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	83





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Sample : K3090-03
Misc :
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Instrument : BNA_G
ClientSampleId : TP-4-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

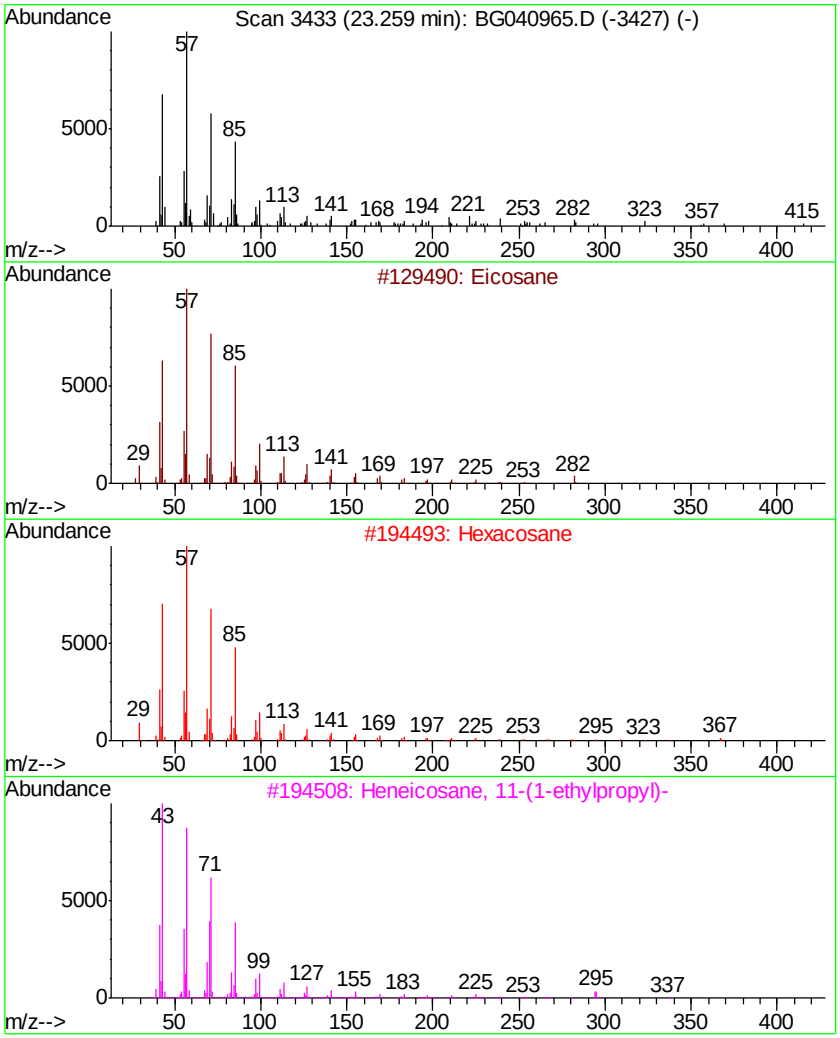
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

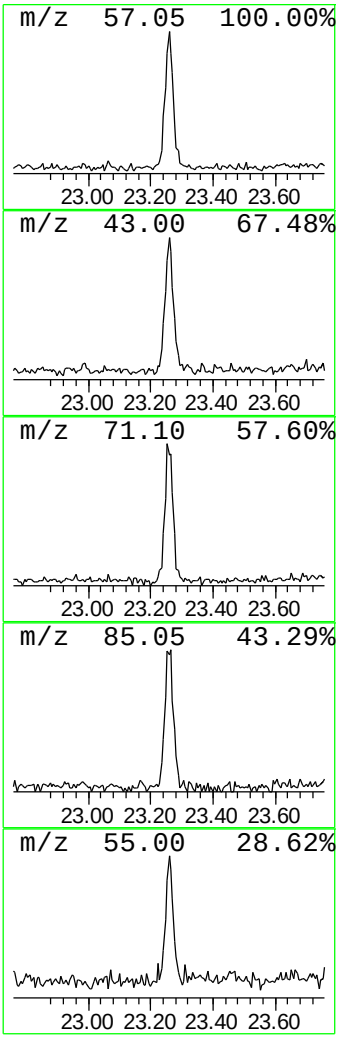
****

Peak Number 8 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.26	2.29 ng	163228	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	Octacosane	394	C28H58	000630-02-4	90
5	Heptacosane	380	C27H56	000593-49-7	90





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Instrument : BNA_G
ClientSampleId : TP-4-S

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

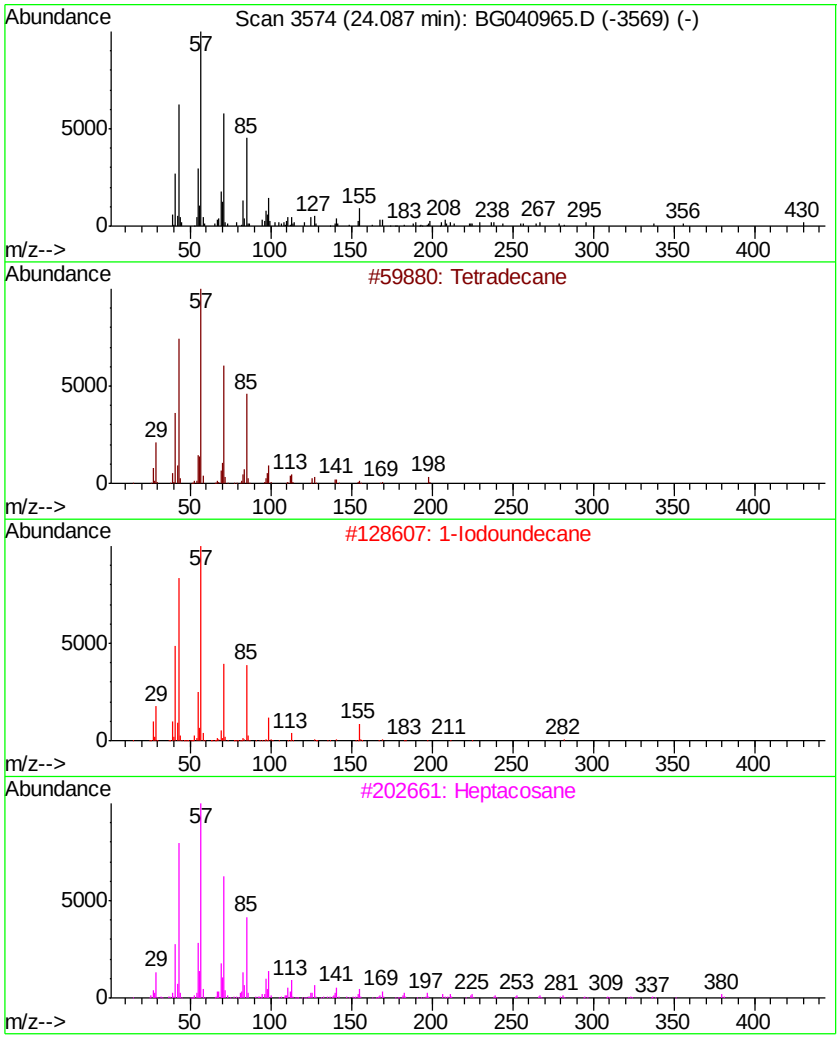
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

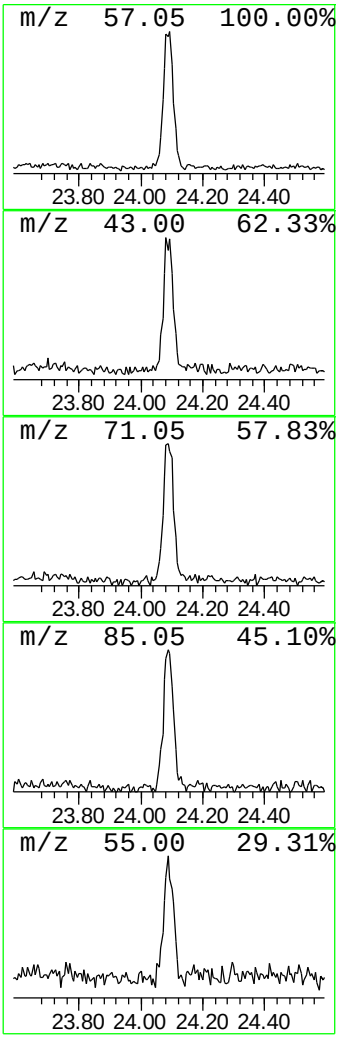
****

Peak Number 9 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.09	2.49 ng	181453	Perylene-d12	25.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	83
2	1-Iodoundecane	282	C11H23I	004282-44-4	83
3	Heptacosane	380	C27H56	000593-49-7	80
4	Octacosane	394	C28H58	000630-02-4	72
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	72





Tentatively Identified Compound (LSC) summary

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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...	3.21	24.5	ng	503080	1	8.12	410728	20.0
unknown7.65	7.65	89.2	ng	1832200	1	8.12	410728	20.0
n-Hexadecanoic acid	18.35	5.8	ng	350596	4	17.49	1205660	20.0
Octadecanoic acid	19.61	2.3	ng	139603	4	17.49	1205660	20.0
Heptadecyl heptaf...	21.37	4.6	ng	326505	5	21.77	1427700	20.0
Eicosane	23.26	2.3	ng	163228	5	21.77	1427700	20.0
Tetradecane	24.09	2.5	ng	181453	6	25.11	1457190	20.0