LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082319\
Data File : BG042436.D
Acq On : 23 Aug 2019 16:51
Operator : HP/JU
Sample : K4086-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-082019

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-BG082219.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	3.116	3	5	31	rVB	841308	1279976	6.87%	1.288%
2	5.560	414	421	438	rBV	1440447	2548805	13.68%	2.564%
3	7.170	686	695	707	rBV	1697418	2858811	15.34%	2.876%
4	7.535	748	757	771	rBV	1888020	3339582	17.92%	3.360%
5	8.005	828	837	845	rBV	534854	953889	5.12%	0.960%
6	8.328	882	892	902	rBV	1304460	2300452	12.35%	2.314%
7	9.168	1021	1035	1047	rBV	841935	1600166	8.59%	1.610%
8	10.825	1307	1317	1330	rBV	834098	1620251	8.70%	1.630%
9	13.281	1727	1735	1746	rBV	3118851	5020974	26.95%	5.051%
10	13.486	1765	1770	1776	rBV2	123063	190102	1.02%	0.191%
11	14.109	1869	1876	1880	rBV	349747	578282	3.10%	0.582%
12	14.556	1947	1952	1957	rBV	218964	310779	1.67%	0.313%
13	14.662	1961	1970	1977	rBV2	1010295	1714448	9.20%	1.725%
14	15.508	2110	2114	2119	rVB	394922	482489	2.59%	0.485%
15	15.919	2173	2184	2189	rBV	191055	439939	2.36%	0.443%
16	16.154	2217	2224	2231	rVV	1541163	2545762	13.66%	2.561%
17	16.371	2257	2261	2264	rBV	519894	749995	4.03%	0.754%
18	17.164	2391	2396	2401	rBV	603855	814637	4.37%	0.820%
19	17.223	2402	2406	2416	rVB2	299423	560776	3.01%	0.564%
20	17.411	2433	2438	2443	rBV2	1159356	1833722	9.84%	1.845%
21	17.452	2443	2445	2451	rVB	317511	446859	2.40%	0.450%
22	17.905	2518	2522	2527	rBV	649542	816229	4.38%	0.821%
23	18.081	2547	2552	2558	rVB	3291205	4251361	22.82%	4.277%
24	18.316	2586	2592	2595	rBV2	607347	870216	4.67%	0.875%
25	18.598	2636	2640	2644	rBV	640465	747230	4.01%	0.752%
26	19.221	2740	2746	2749	rBV	6971249	10267567	55.10%	10.329%
27	19.262	2749	2753	2762	rVB	12365507	18633092	100.00%	18.744%
28	19.380	2769	2773	2779	rVB	1637287	2037489	10.93%	2.050%
29	19.468	2780	2788	2795	rBV	1822423	2992769	16.06%	3.011%
30	19.738	2832	2834	2839	rVB2	281075	318379	1.71%	0.320%
31	19.803	2841	2845	2847	rVV2	686419	900053	4.83%	0.905%
32	19.832	2847	2850	2857	rVB	1118995	1644020	8.82%	1.654%
33	19.926	2864	2866	2872	rBV5	119107	247179	1.33%	0.249%
34	20.032	2878	2884	2889	rVB	3807141	5223832	28.04%	5.255%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082319\
Data File : BG042436.D
Acq On : 23 Aug 2019 16:51
Operator : HP/JU
Sample : K4086-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-082019

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-BG082219.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.331	2932	2935	2938	rBV4	430662	665163	3.57%	0.669%
36	20.361	2938	2940	2948	rVB3	648346	809077	4.34%	0.814%
37	20.472	2955	2959	2964	rBV3	536589	856660	4.60%	0.862%
38	20.631	2982	2986	2989	rBV3	267568	375724	2.02%	0.378%
39	20.831	3016	3020	3024	rBV	325343	413017	2.22%	0.415%
40	21.230	3084	3088	3090	rBV4	185434	279457	1.50%	0.281%
41	21.348	3104	3108	3116	rVB4	433845	795247	4.27%	0.800%
42	21.495	3129	3133	3137	rVB	389339	490111	2.63%	0.493%
43	21.694	3159	3167	3171	rBV3	1366513	3381979	18.15%	3.402%
44	21.736	3172	3174	3184	rVB	724138	1142224	6.13%	1.149%
45	21.894	3197	3201	3206	rVB	358231	446262	2.39%	0.449%
46	22.053	3226	3228	3229	rBV2	196421	203207	1.09%	0.204%
47	22.505	3301	3305	3311	rVV3	479468	888073	4.77%	0.893%
48	22.576	3315	3317	3323	rVB5	309966	274571	1.47%	0.276%
49	22.793	3351	3354	3358	rBV5	228501	529991	2.84%	0.533%
50	23.704	3508	3509	3514	rVB3	233805	206986	1.11%	0.208%
51	23.904	3541	3543	3544	rBV	429524	312863	1.68%	0.315%
52	24.027	3561	3564	3573	rVB	727670	1384121	7.43%	1.392%
53	24.462	3635	3638	3644	rVB4	289293	358829	1.93%	0.361%
54	24.879	3707	3709	3712	rBV3	223556	234859	1.26%	0.236%
55	25.308	3778	3782	3791	rBV4	417078	1340477	7.19%	1.348%
56	25.948	3889	3891	3893	rBV2	216914	259298	1.39%	0.261%
57	26.136	3921	3923	3926	rBV	281803	224531	1.21%	0.226%
58	26.783	4031	4033	4040	rBV4	259858	550896	2.96%	0.554%
59	27.259	4112	4114	4115	rBV2	224067	228352	1.23%	0.230%
60	27.517	4153	4158	4167	rBV5	327020	1249859	6.71%	1.257%
61	28.504	4323	4326	4328	rBV2	283599	363813	1.95%	0.366%

Sum of corrected areas: 99405759

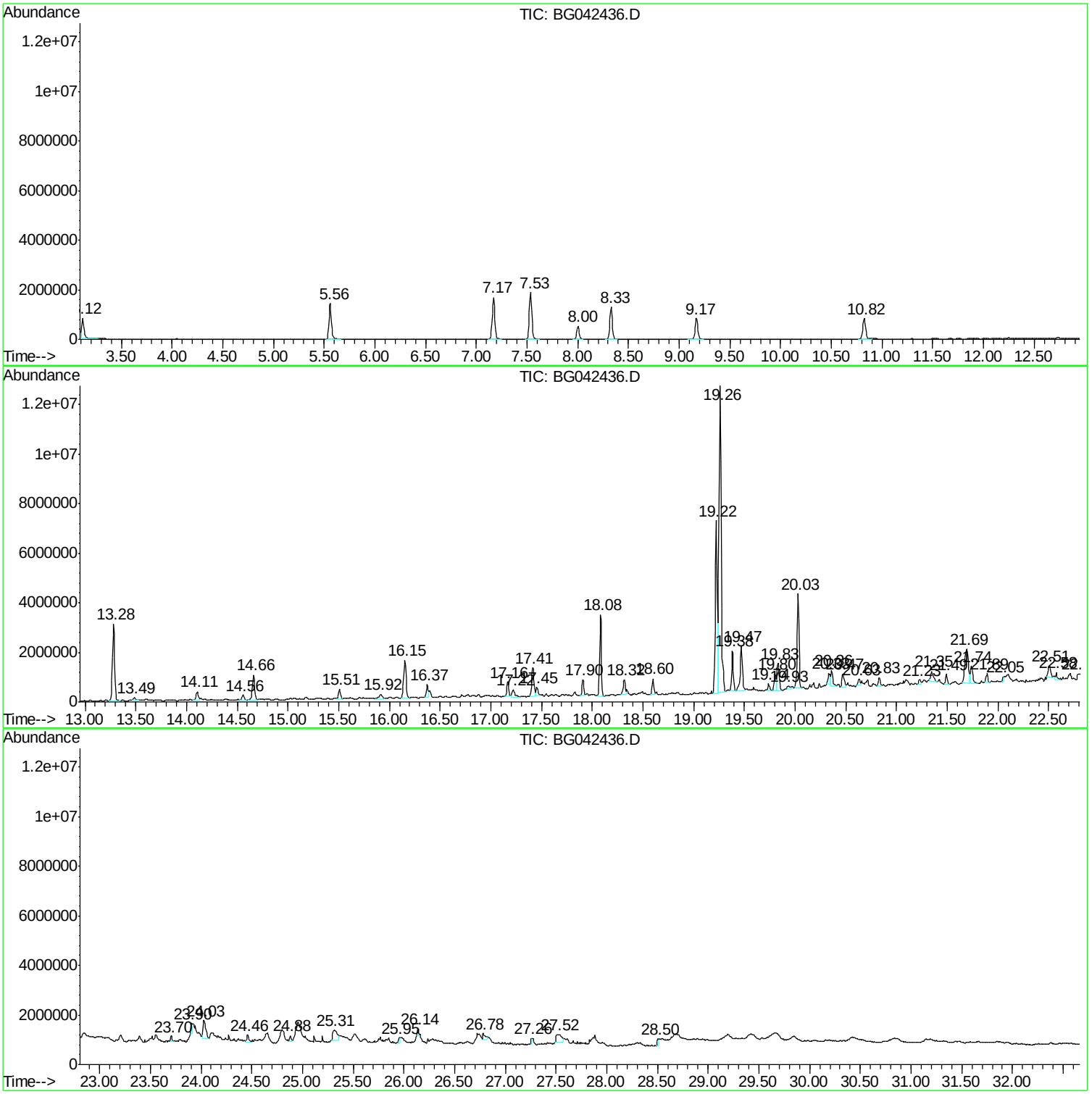
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082319\
Data File : BG042436.D
Acq On : 23 Aug 2019 16:51
Operator : HP/JU
Sample : K4086-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-082019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.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\BG082319\
Data File : BG042436.D
Acq On : 23 Aug 2019 16:51
Operator : HP/JU
Sample : K4086-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-082019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

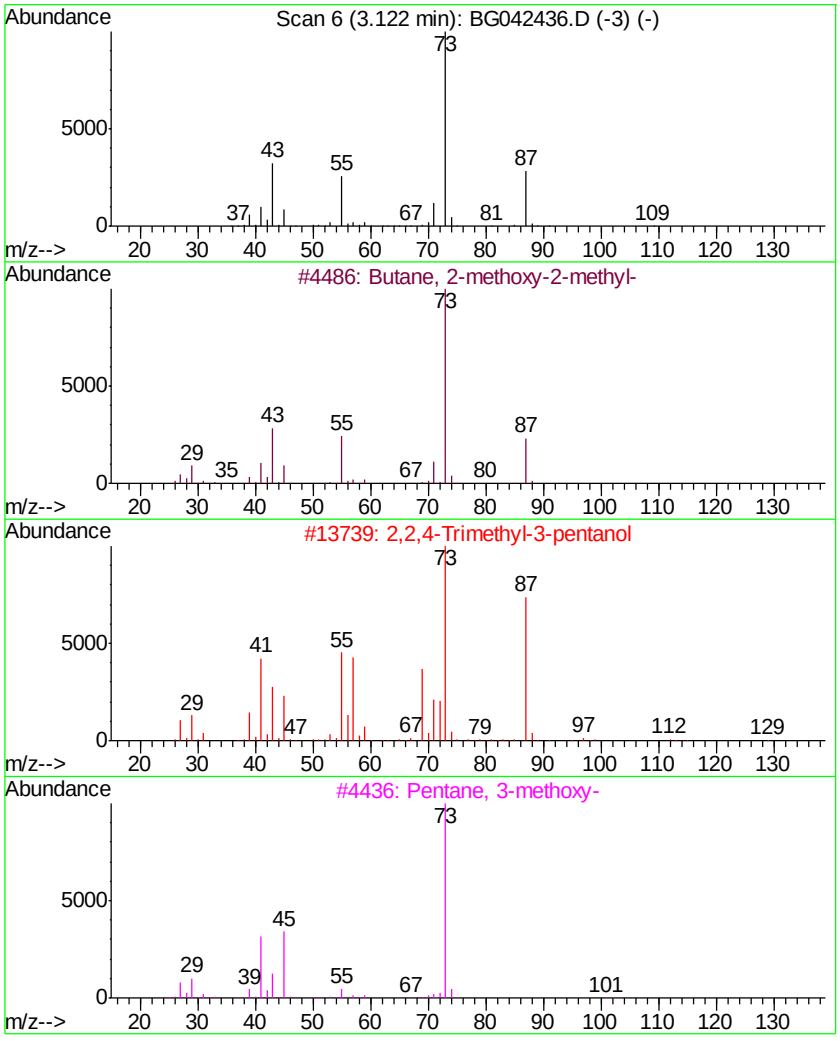
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

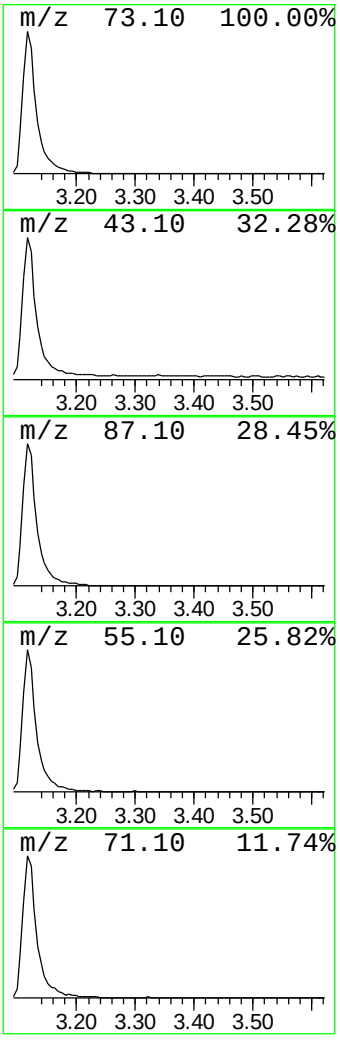
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	26.84 ng	1279980	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082319\
Data File : BG042436.D
Acq On : 23 Aug 2019 16:51
Operator : HP/JU
Sample : K4086-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-082019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

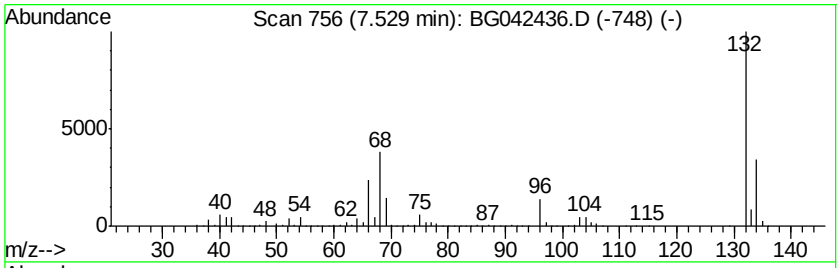
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

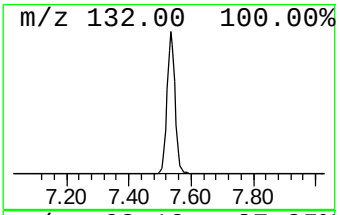
****

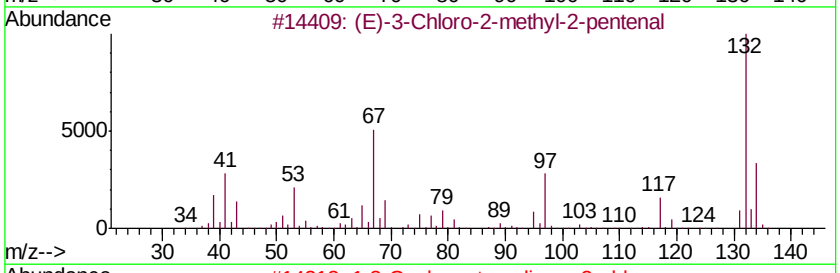
Peak Number 2 unknown7.53 Concentration Rank 5

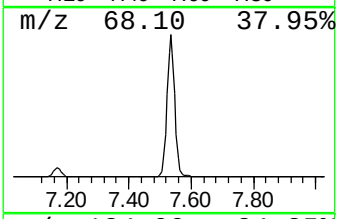
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	70.02 ng	3339580	1,4-Dichlorobenzene-d4	8.00

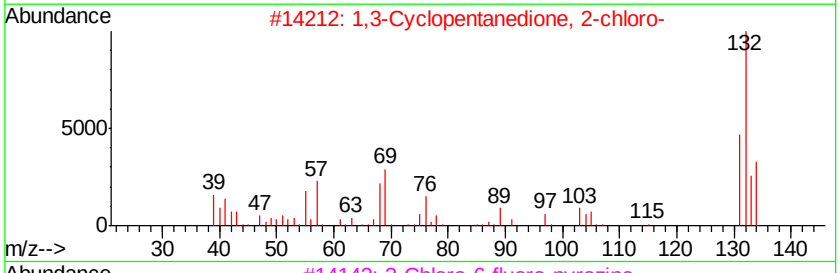
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	38
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	32
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
5	1-Isoquinolinemethanol, .alpha.-...	191	C12H17NO	114608-92-3	12

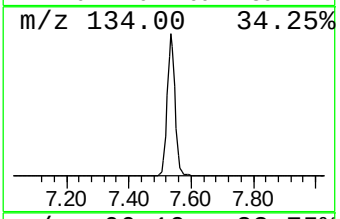


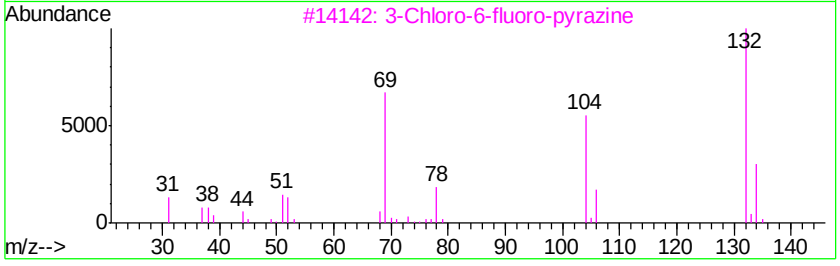


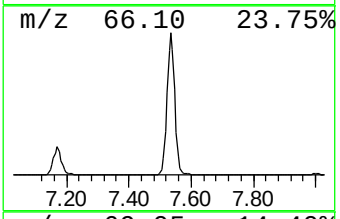


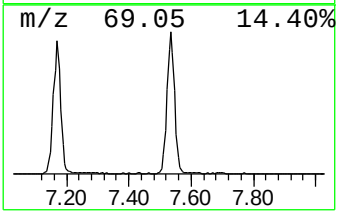












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Misc :
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Instrument : BNA_G
ClientSampleId : NB-08-082019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

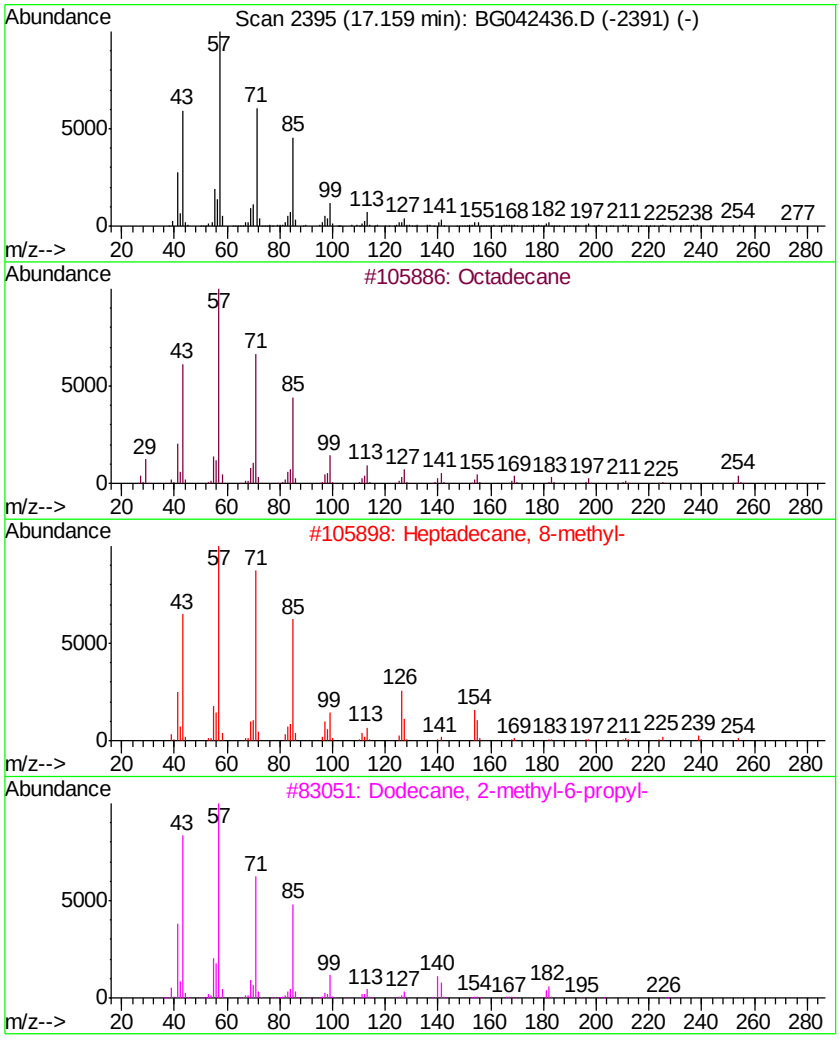
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

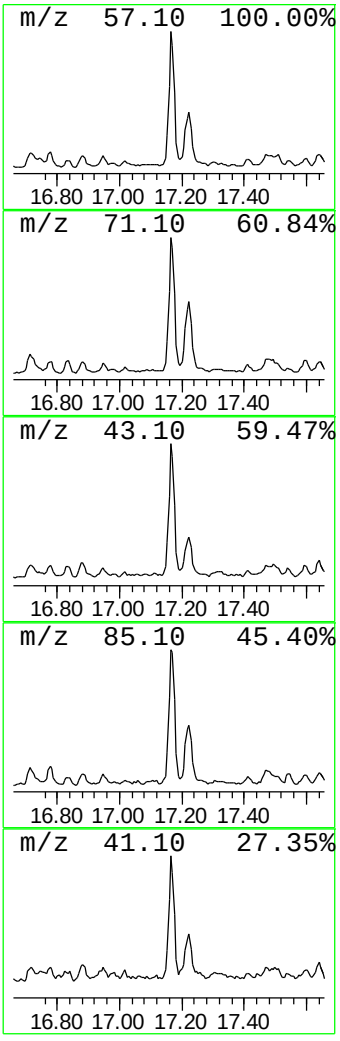
****

Peak Number 4 Octadecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	8.89 ng	814637	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	94
2	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	94
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	93
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	90





Library Search Compound Report

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Data File : BG042436.D
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Instrument : BNA_G
ClientSampleId : NB-08-082019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

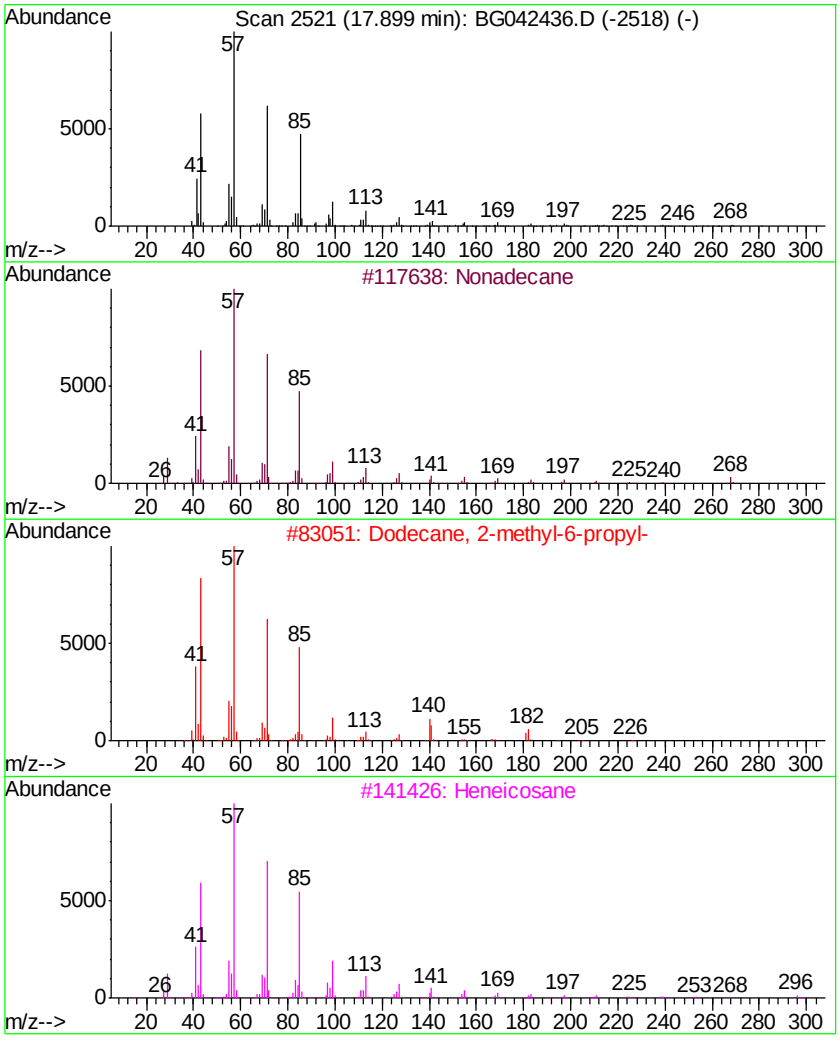
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

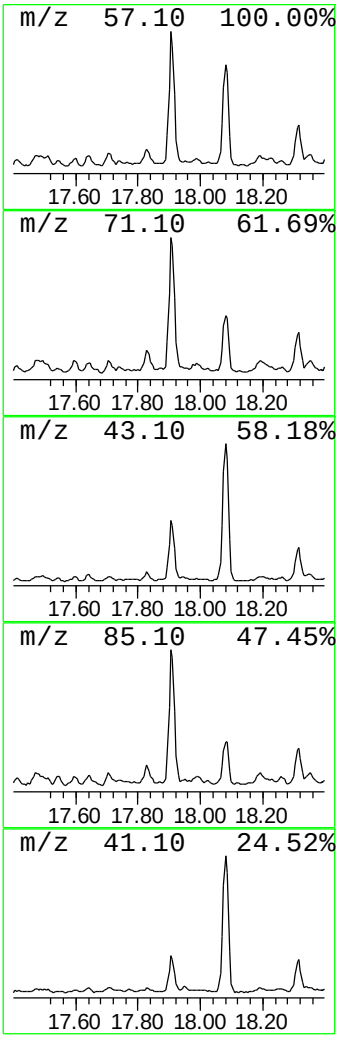
****

Peak Number 5 Nonadecane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.90	8.90 ng	816229	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	97
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Eicosane	282	C20H42	000112-95-8	90
5	Heptadecane	240	C17H36	000629-78-7	87





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Data File : BG042436.D
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Misc :
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Instrument : BNA_G
ClientSampleId : NB-08-082019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

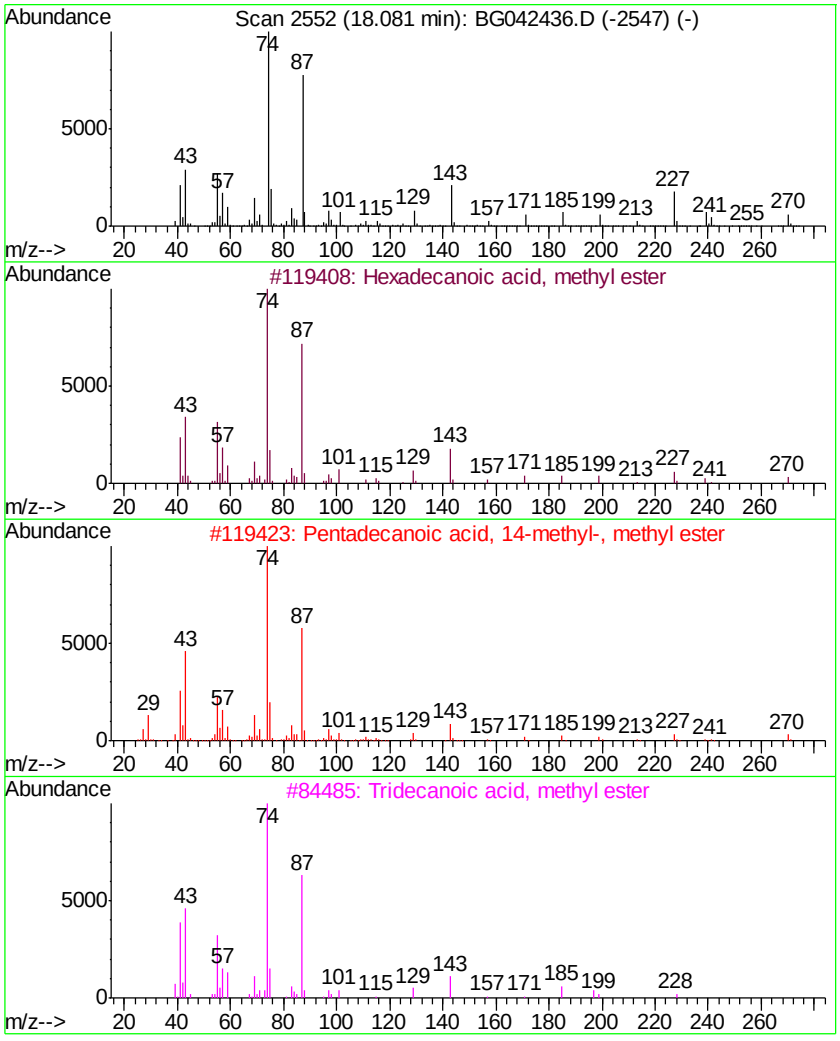
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

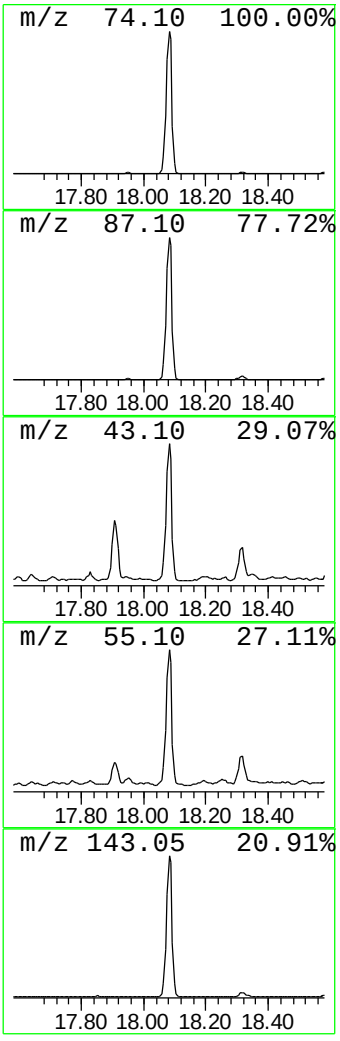
****

Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.08	46.37 ng	4251360	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082319\
Data File : BG042436.D
Acq On : 23 Aug 2019 16:51
Operator : HP/JU
Sample : K4086-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-082019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

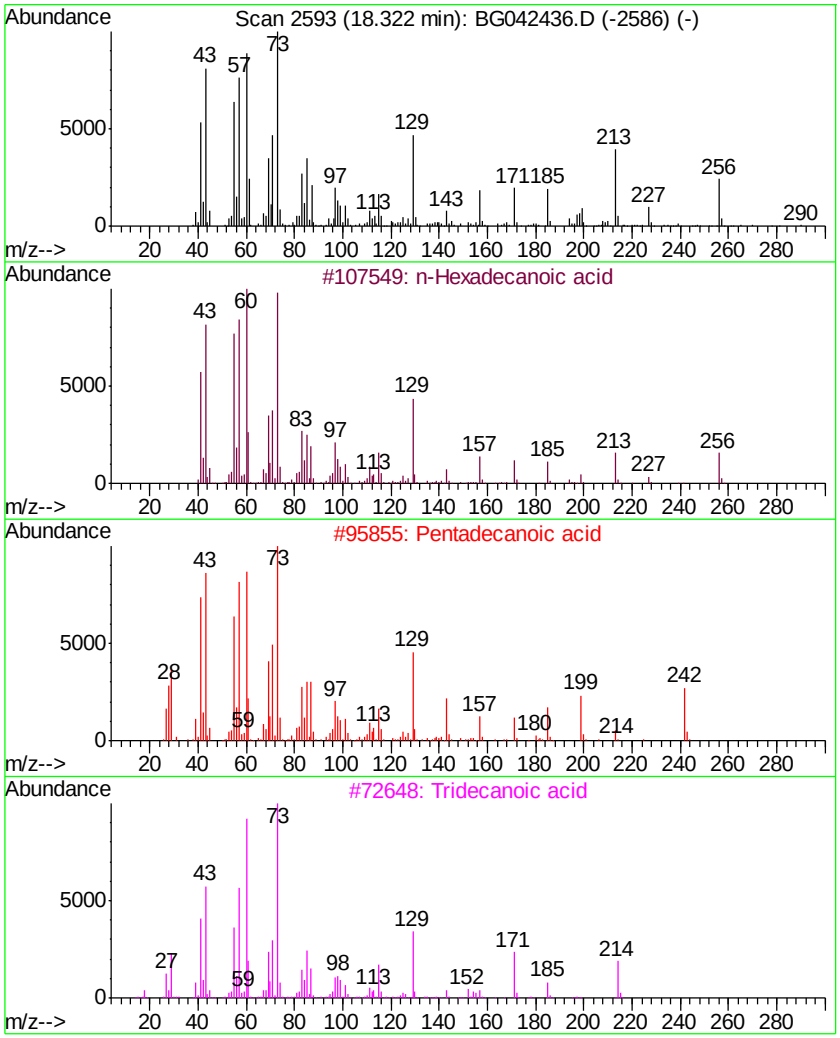
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

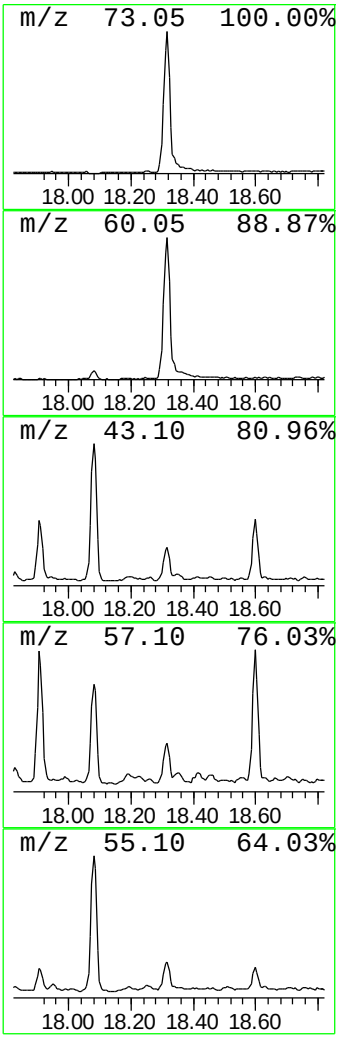
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	9.49 ng	870216	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Dodecane, 5,8-diethyl-	226	C16H34	024251-86-3	25





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Acq On : 23 Aug 2019 16:51
Operator : HP/JU
Sample : K4086-01
Misc :
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Instrument : BNA_G
ClientSampleId : NB-08-082019

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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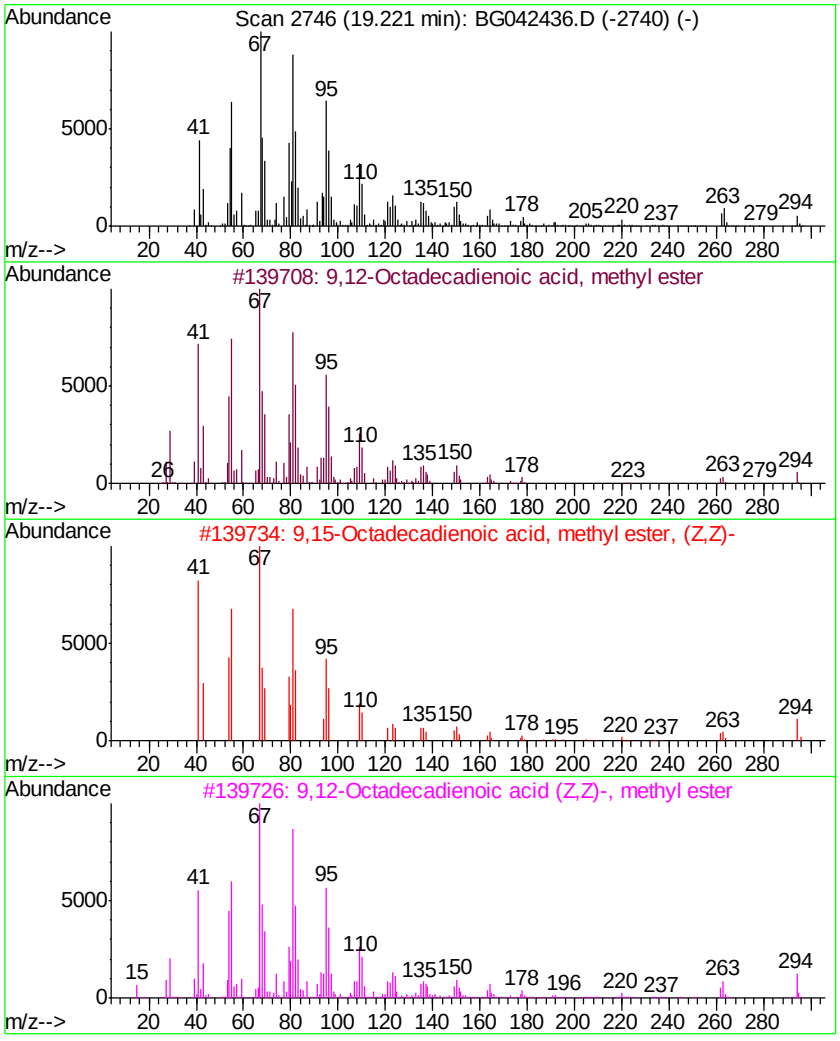
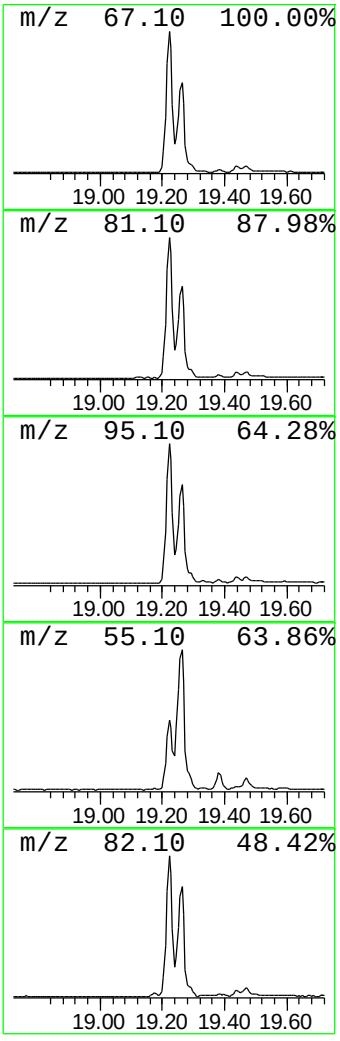
Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.22	111.99 ng	10267600	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : NB-08-082019

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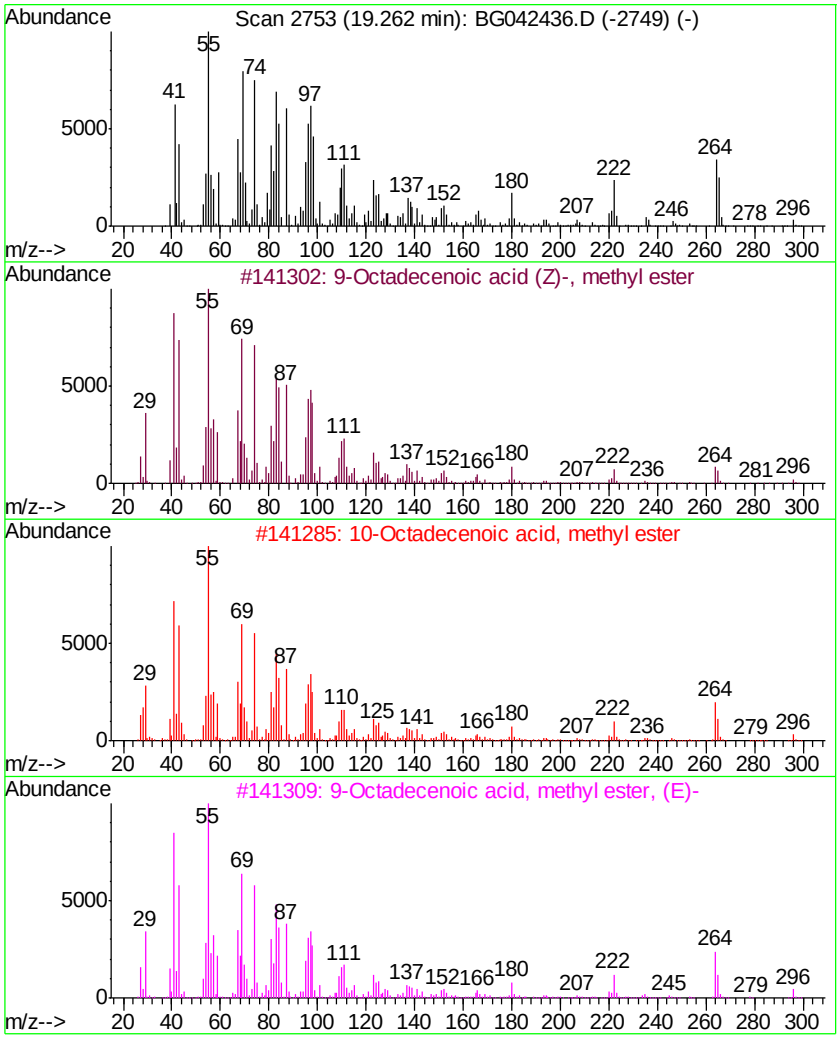
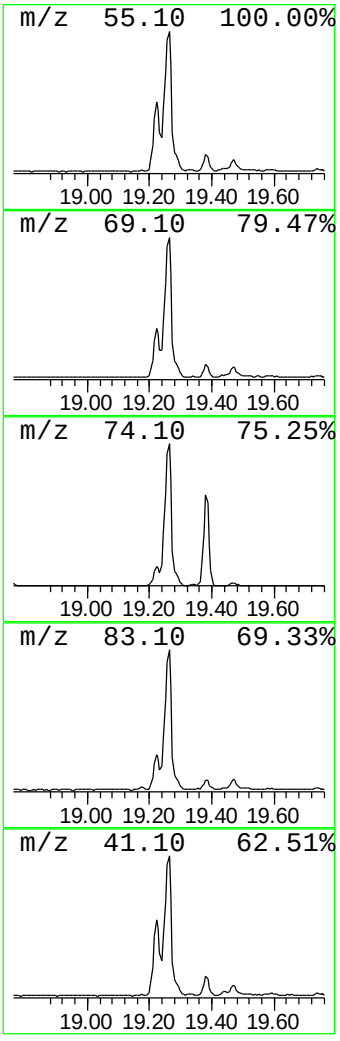
Peak Number 9 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.26	203.23 ng	18633100	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99





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Instrument : BNA_G
ClientSampleId : NB-08-082019

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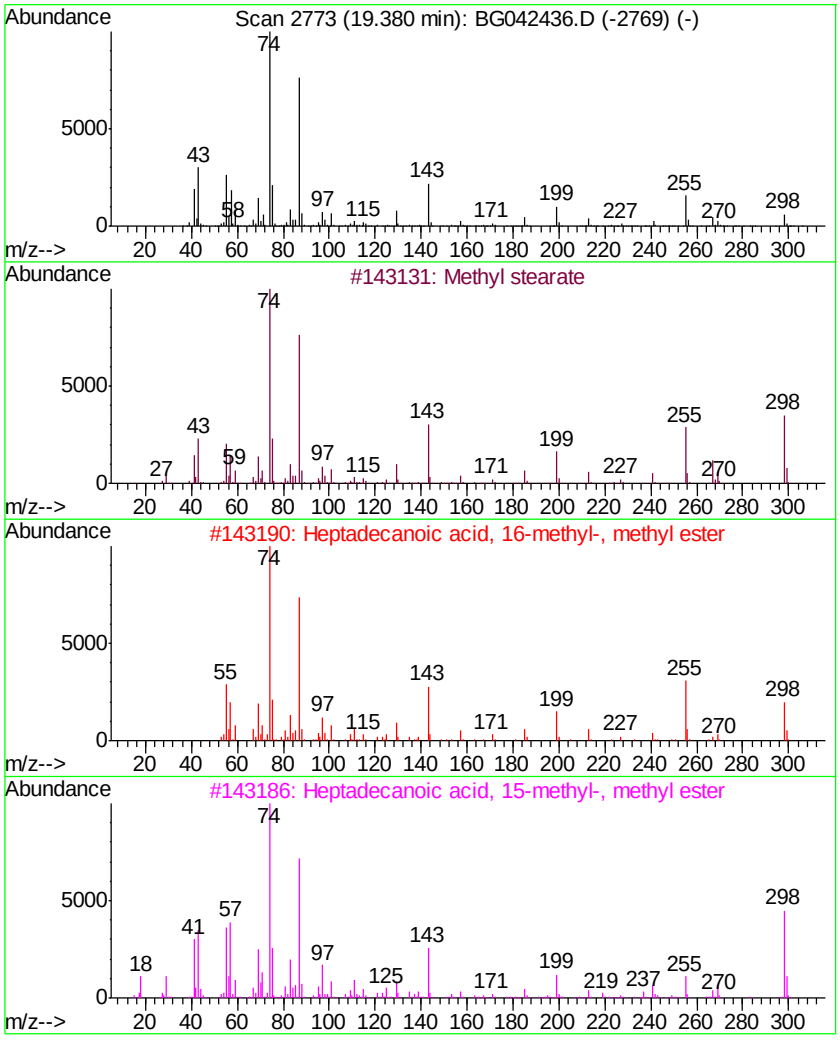
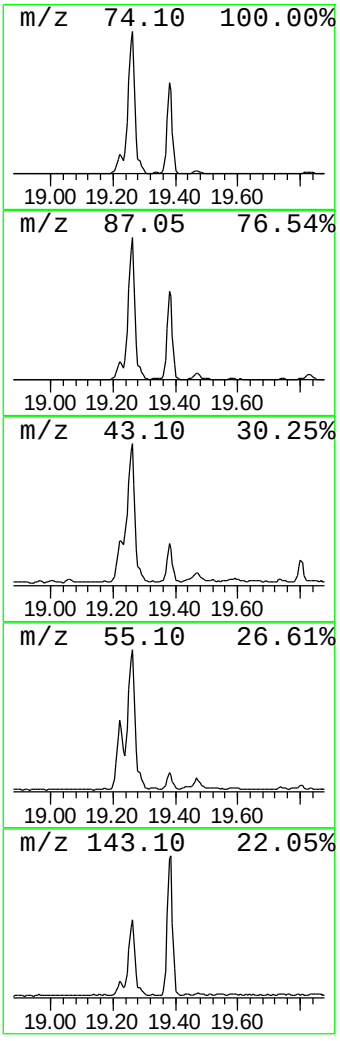
Peak Number 10 Methyl stearate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.38	22.22 ng	2037490	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	91
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90





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ClientSampleId : NB-08-082019

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Peak Number 11 1-Bromo-11-iodoundecane Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.70	17.63 ng	206986	Perylene-d12	24.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Bromo-11-iodoundecane	360	C11H22BrI	139123-69-6	56
2	9-Undecen-2-one, 6,10-dimethyl-	196	C13H24O	004433-36-7	55
3	Cyclotetradecane, 1,7,11-trimeth...	280	C20H40	001786-12-5	45
4	Silane, dimethyl(2,2,2-trichloro...	404	C17H35Cl3O2Si	1000347-56-9	38
5	3-Buten-2-one, 3-methyl-4-(1,3,3...	222	C14H22O2	097371-44-3	38