LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043485.D
Acq On : 4 Nov 2019 17:50
Operator : JU
Sample : K5623-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAT-TOTE

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-BG102119.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	3.181	10	16	29	rVB	732791	1321351	43.07%	6.312%
2	5.114	339	345	353	rBV	85483	138809	4.52%	0.663%
3	5.602	420	428	442	rBV	506641	905212	29.51%	4.324%
4	7.200	691	700	718	rBV2	362707	831860	27.12%	3.973%
5	7.553	750	760	772	rBV	731420	1335543	43.53%	6.379%
6	8.011	831	838	846	rBV2	172676	299686	9.77%	1.431%
7	8.334	886	893	904	rBV	561588	1013308	33.03%	4.840%
8	9.174	1028	1036	1047	rBV	389769	764332	24.91%	3.651%
9	10.814	1308	1315	1327	rBV	198348	396553	12.93%	1.894%
10	11.577	1439	1445	1456	rBV2	181227	537008	17.50%	2.565%
11	13.264	1723	1732	1741	rBV	1239785	1999669	65.18%	9.552%
12	14.016	1857	1860	1865	rBV4	19886	39919	1.30%	0.191%
13	14.092	1867	1873	1884	rVB	340098	535879	17.47%	2.560%
14	14.639	1960	1966	1975	rVB2	371471	586282	19.11%	2.800%
15	15.009	2025	2029	2035	rBV5	24144	34368	1.12%	0.164%
16	15.925	2181	2185	2190	rBV	18108	30793	1.00%	0.147%
17	16.131	2213	2220	2233	rBV	1094241	1779541	58.01%	8.500%
18	17.388	2427	2434	2443	rBV	423537	689091	22.46%	3.292%
19	18.046	2543	2546	2551	rVB7	30364	39772	1.30%	0.190%
20	18.287	2581	2587	2600	rBV	576992	943948	30.77%	4.509%
21	18.493	2619	2622	2630	rVB2	29935	48441	1.58%	0.231%
22	19.239	2746	2749	2753	rVB3	26626	30965	1.01%	0.148%
23	19.550	2797	2802	2812	rBV	276589	413589	13.48%	1.976%
24	19.997	2873	2878	2888	rBV	2343729	3067781	100.00%	14.654%
25	21.295	3094	3099	3109	rBV	312270	513197	16.73%	2.451%
26	21.654	3154	3160	3170	rBV	461602	781355	25.47%	3.732%
27	22.441	3291	3294	3299	rVB2	57717	81137	2.64%	0.388%
28	23.129	3405	3411	3416	rBV	102494	194917	6.35%	0.931%
29	23.916	3540	3545	3553	rBV3	108601	240263	7.83%	1.148%
30	24.856	3696	3705	3718	rVB3	401849	1116482	36.39%	5.333%
31	25.966	3890	3894	3904	rVB2	80982	224239	7.31%	1.071%

Sum of corrected areas: 20935290

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043485.D
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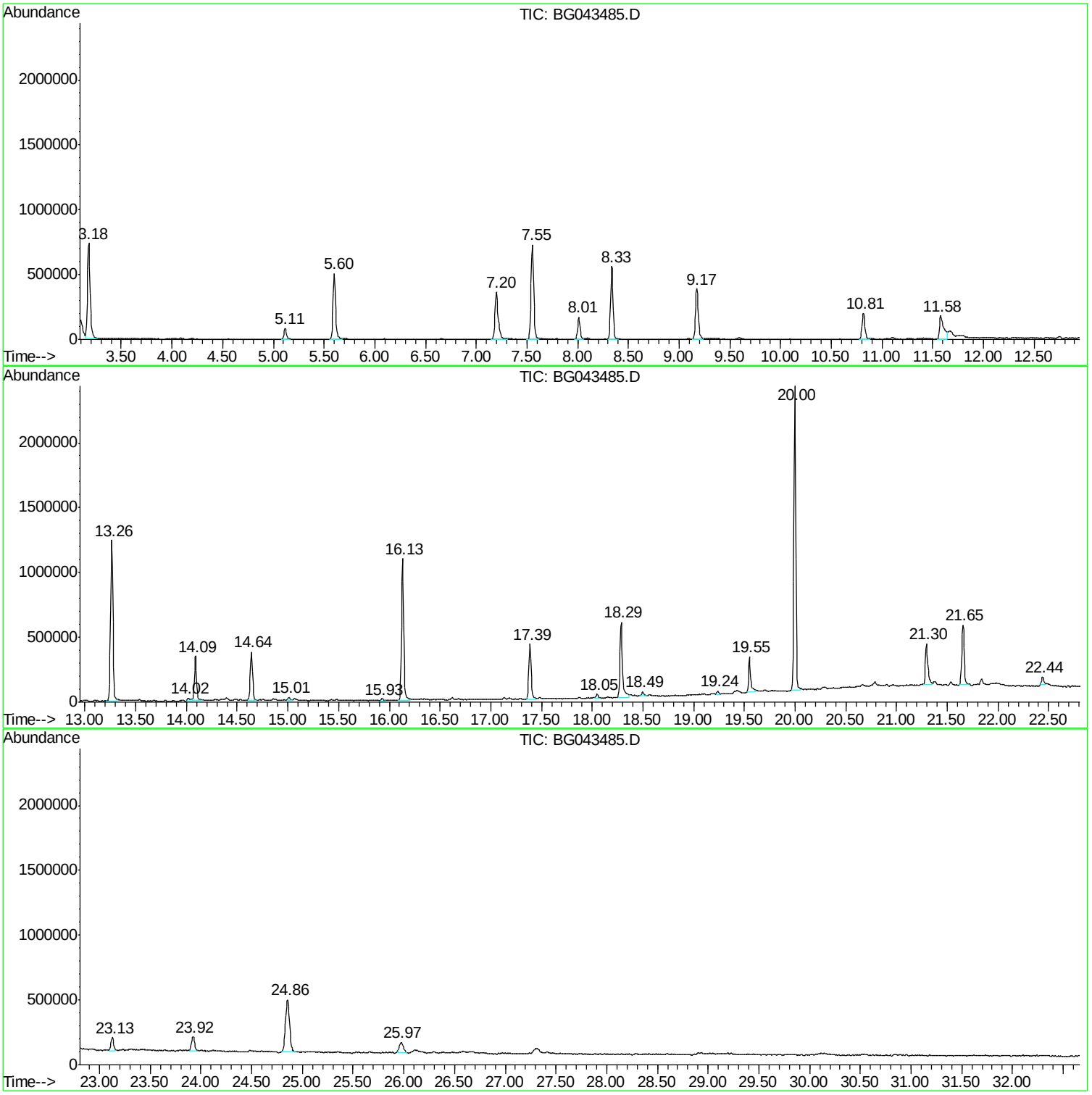
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAT-TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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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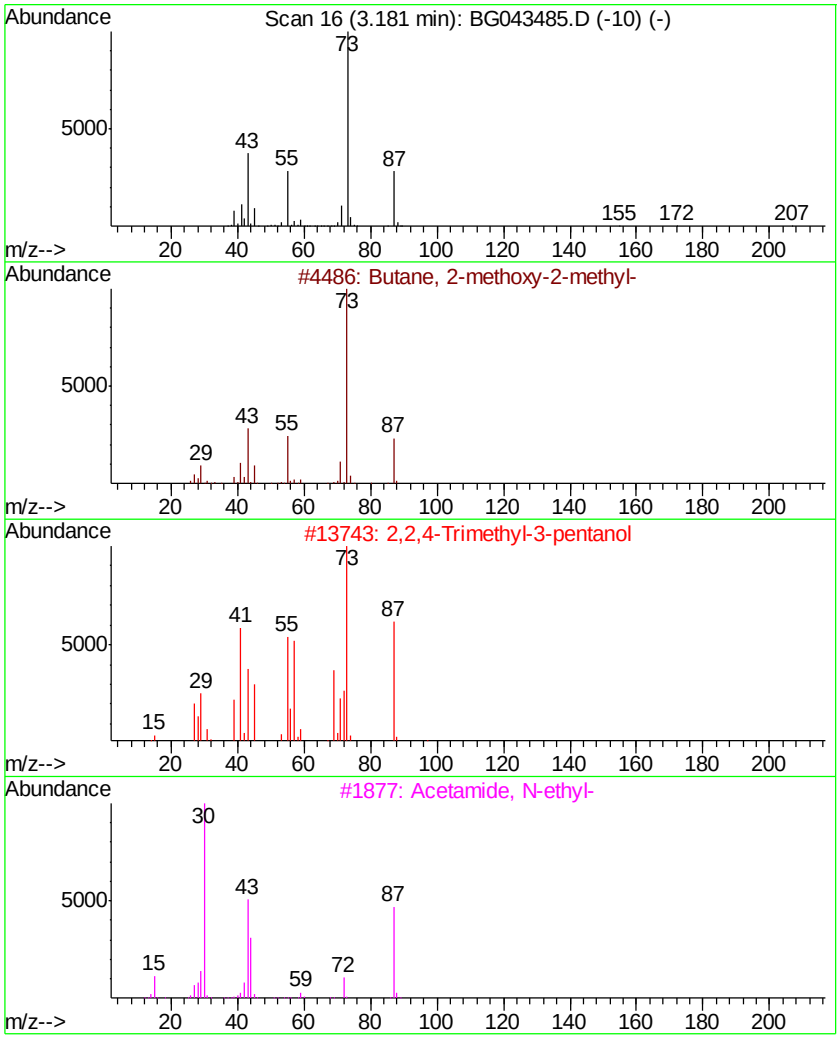
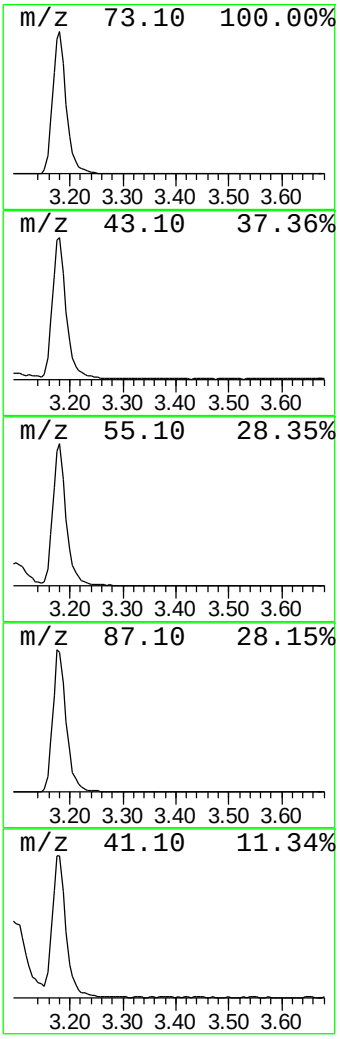
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	88.18 ng	1321350	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Sample : K5623-02
Misc :
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Instrument : BNA_G
ClientSampleId : PAT-TOTE

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

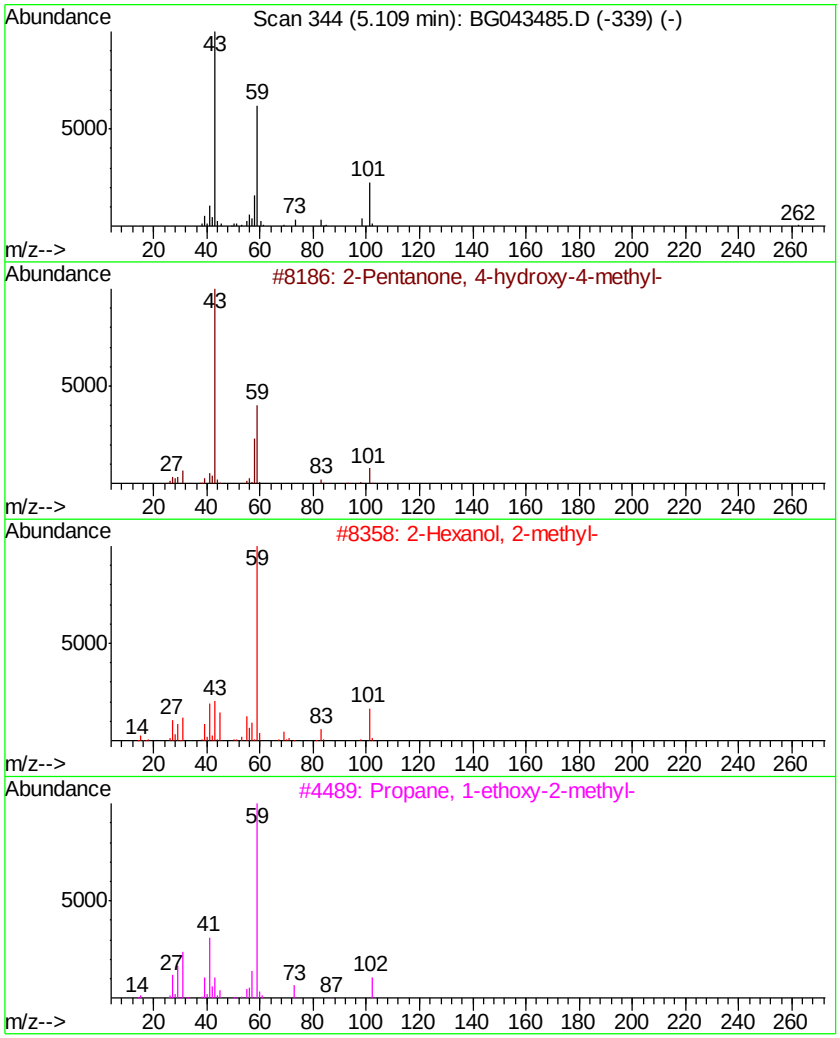
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

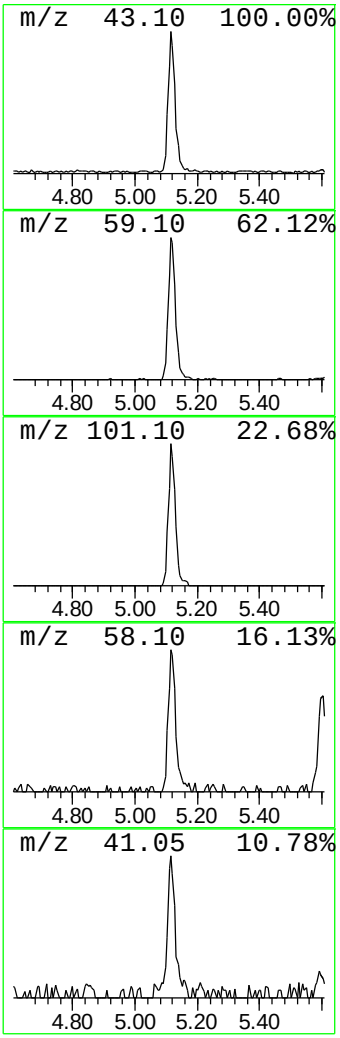
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	9.26 ng	138809	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	2-Pentanol, 5-methoxy-2-methyl-	132	C7H16O2	055724-04-4	23





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : PAT-TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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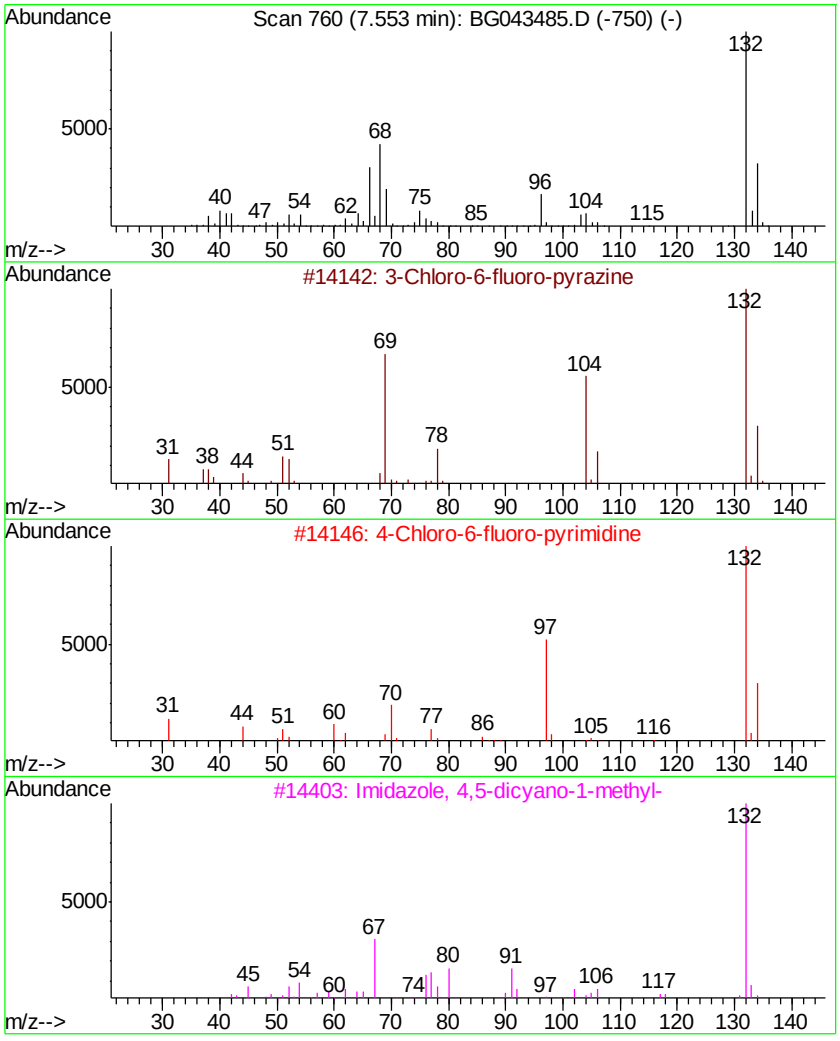
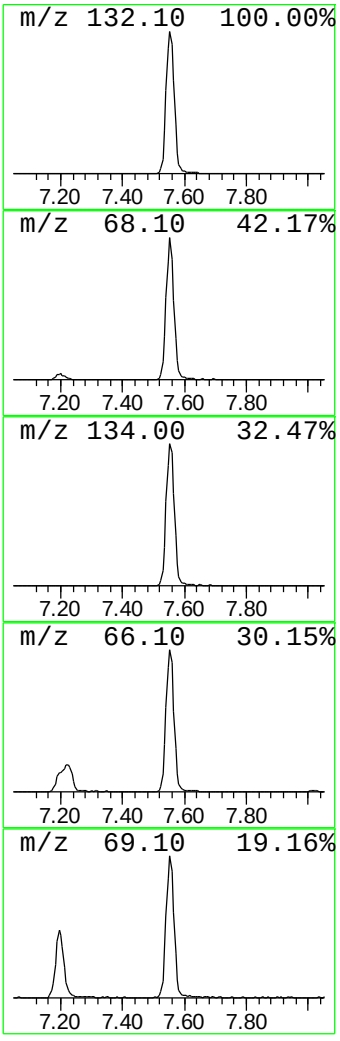
****

Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	89.13 ng	1335540	1,4-Dichlorobenzene-d4	8.01

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	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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Operator : JU
Sample : K5623-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAT-TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

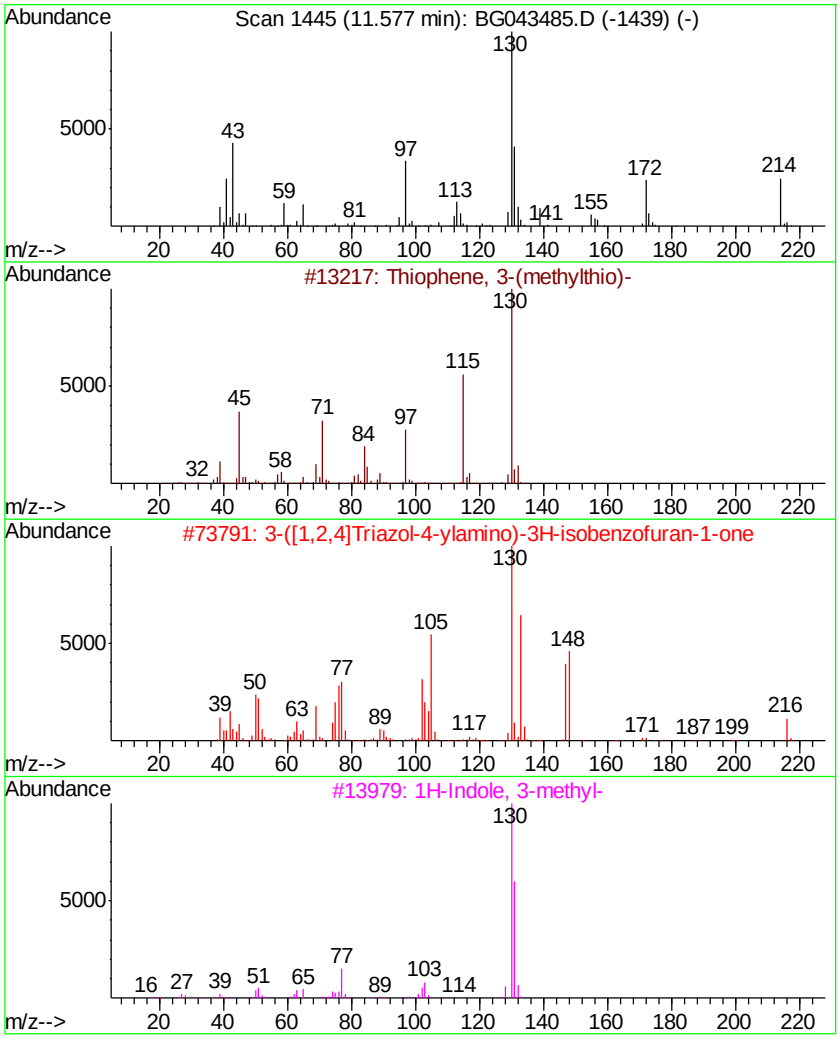
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

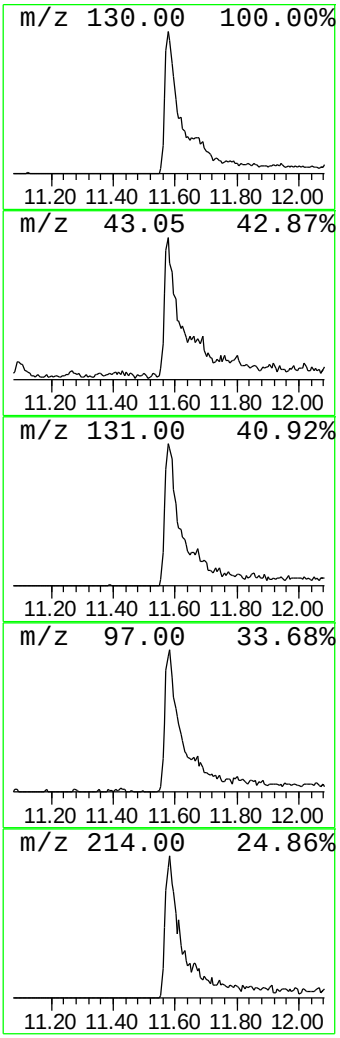
****

Peak Number 5 unknown11.58 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	27.08 ng	537008	Naphthalene-d8	10.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 3-(methylthio)-	130	C5H6S2	020731-74-2	32
2	3-([1,2,4]Triazol-4-ylamino)-3H-...	216	C10H8N4O2	1000300-48-4	30
3	1H-Indole, 3-methyl-	131	C9H9N	000083-34-1	28
4	Methamphetamine, N-trimethylsilyl-	221	C13H23NSi	1000297-92-8	25
5	Carbonic acid, butyl 3,5-difluop...	230	C11H12F2O3	1000357-84-1	17





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Misc :
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Instrument : BNA_G
ClientSampleId : PAT-TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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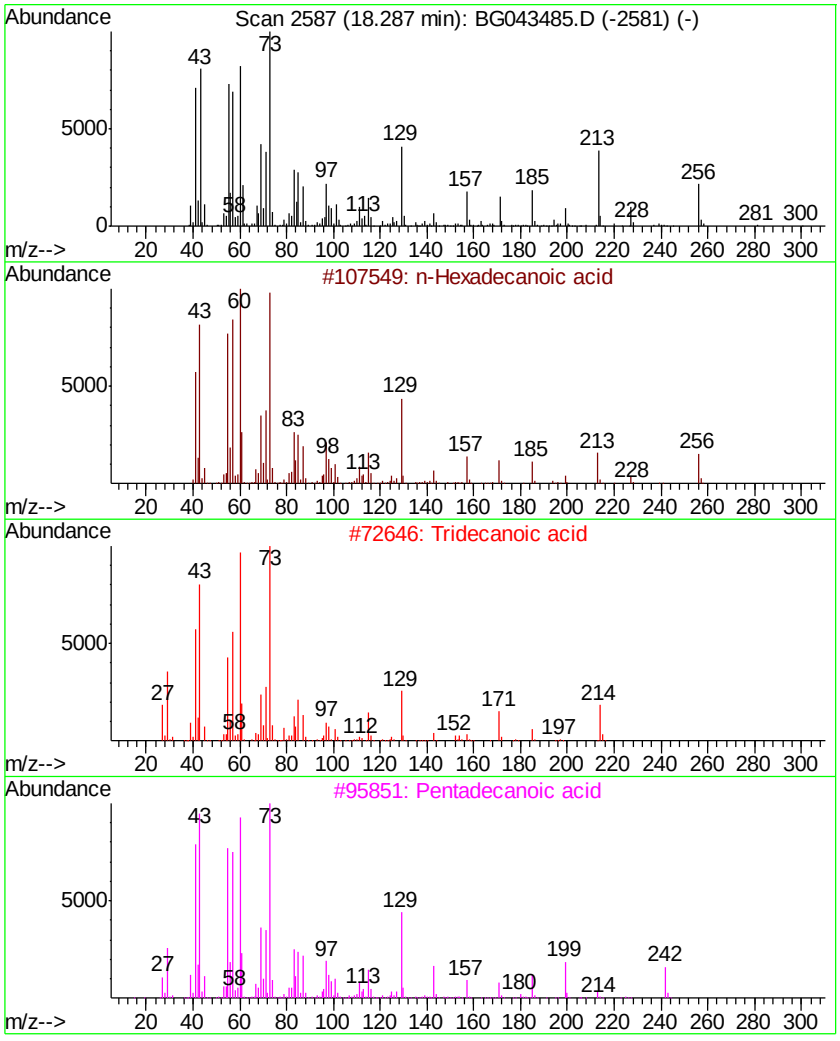
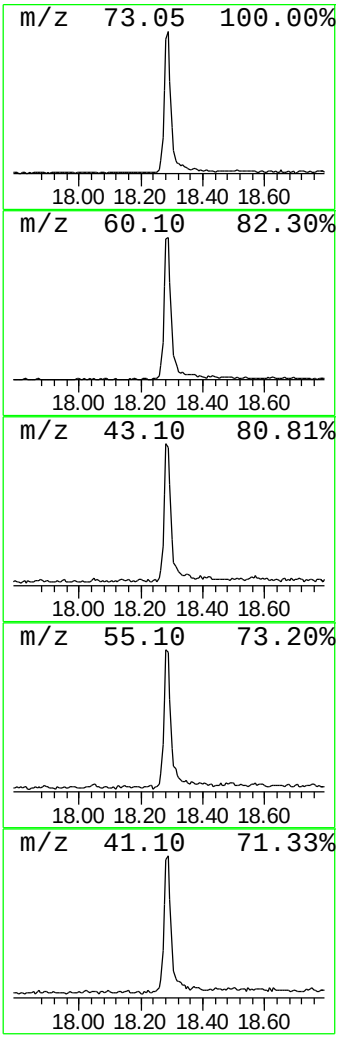
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	27.40 ng	943948	Phenanthrene-d10	17.39

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	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Instrument : BNA_G
ClientSampleId : PAT-TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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TIC Library : C:\Database\NIST11.L
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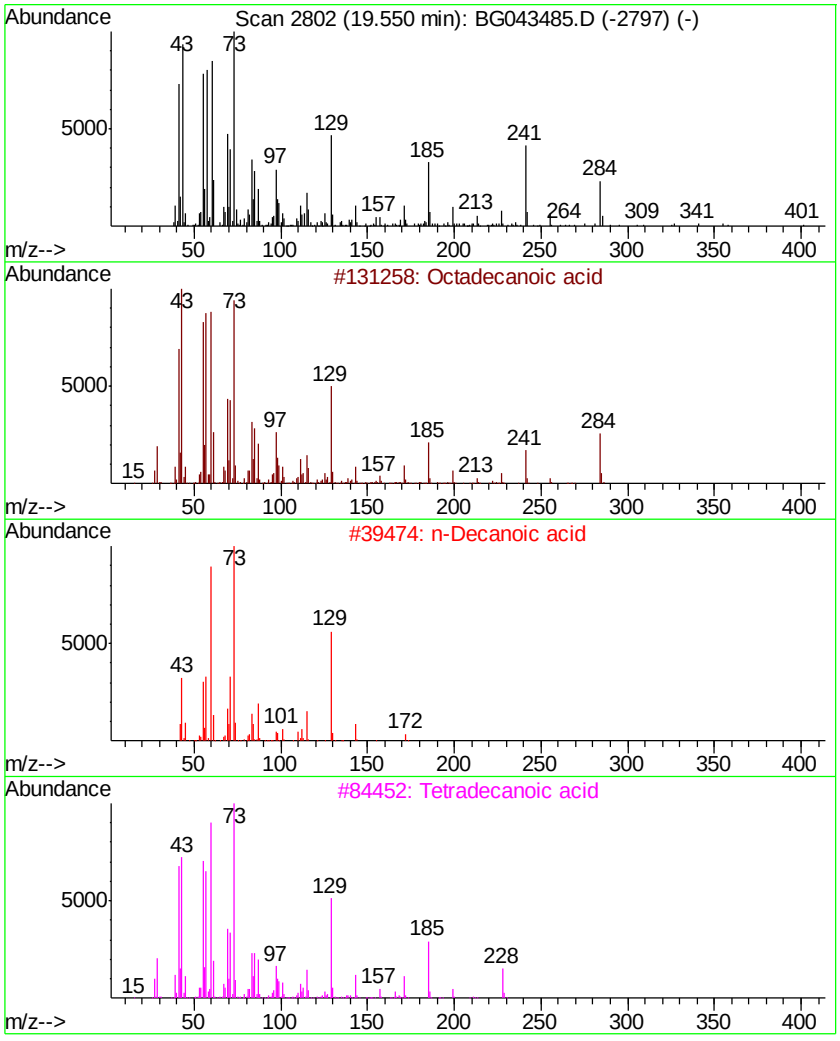
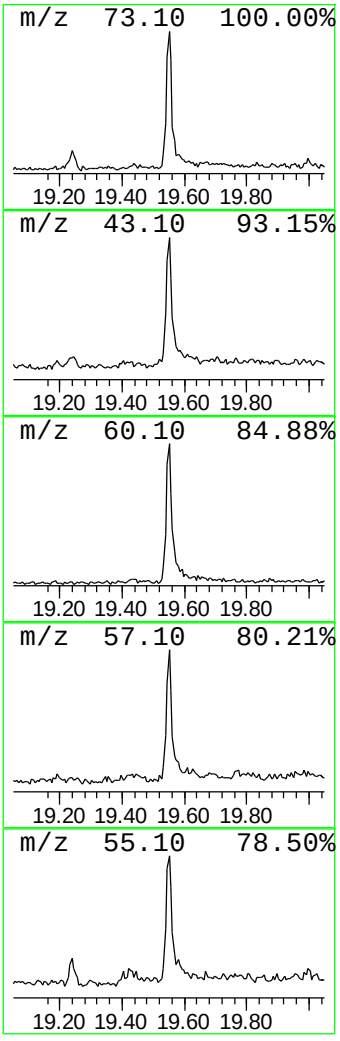
Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.55	10.59 ng	413589	Chrysene-d12	21.65

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	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64





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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

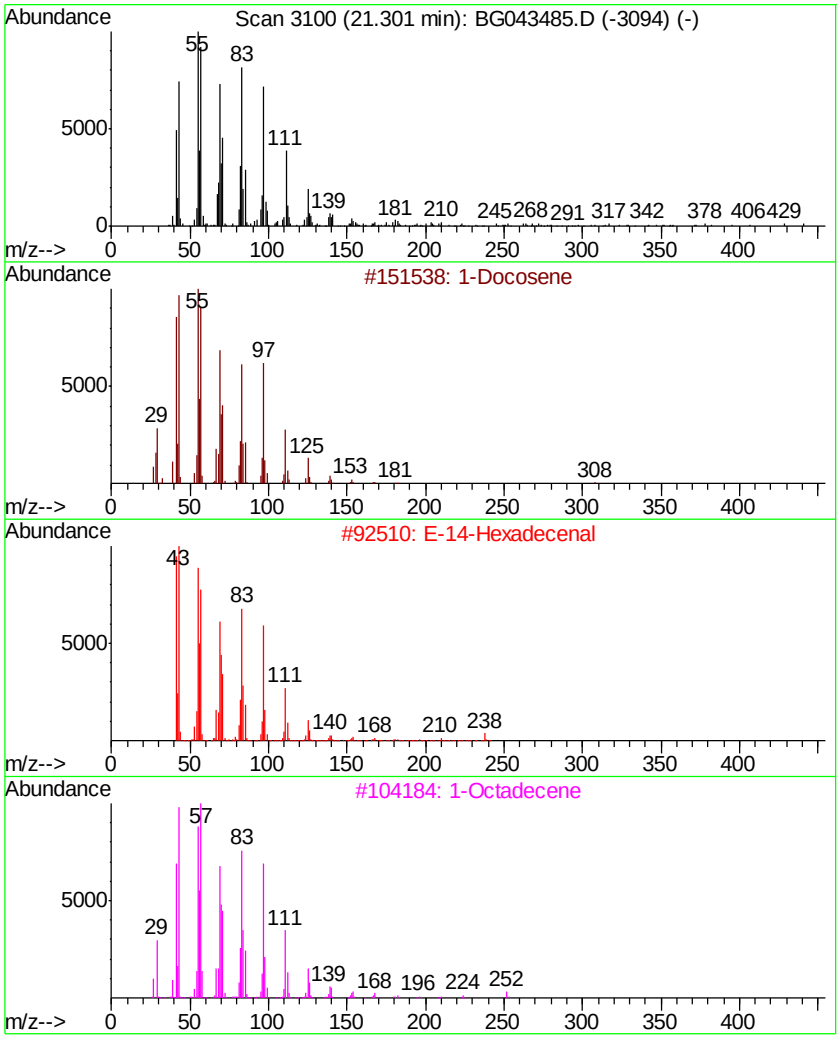
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

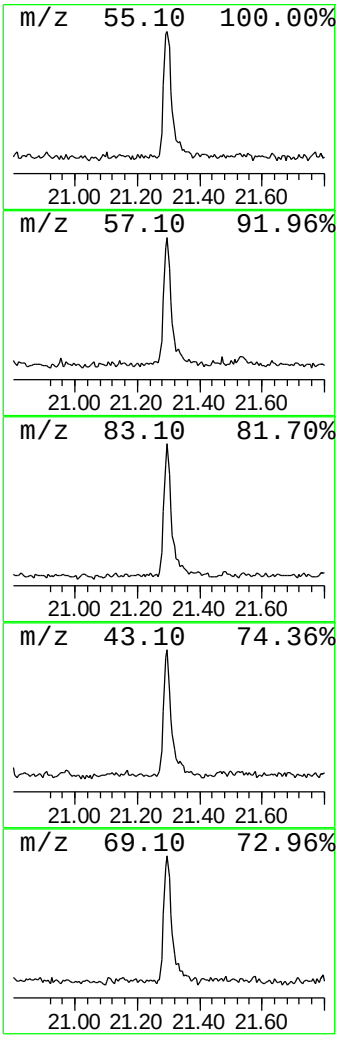
****

Peak Number 8 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	13.14 ng	513197	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	98
2	E-14-Hexadecenal	238	C16H30O	330207-53-9	97
3	1-Octadecene	252	C18H36	000112-88-9	96
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
5	1-Tricosene	322	C23H46	018835-32-0	95





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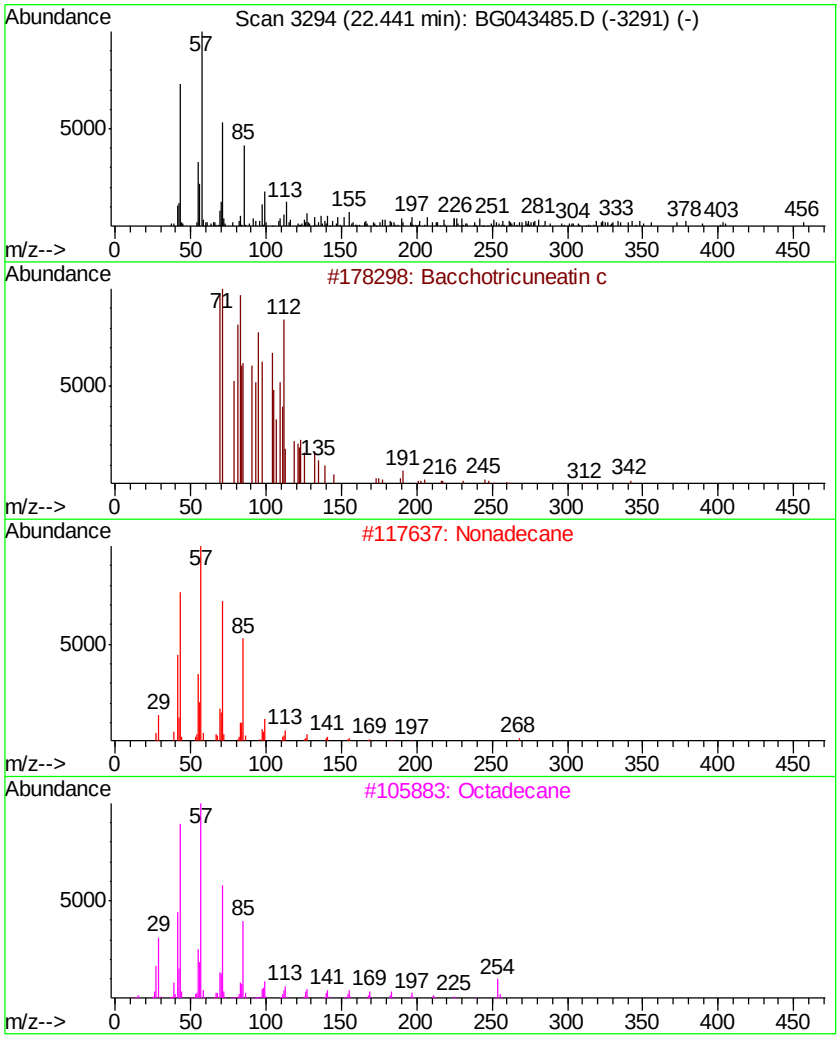
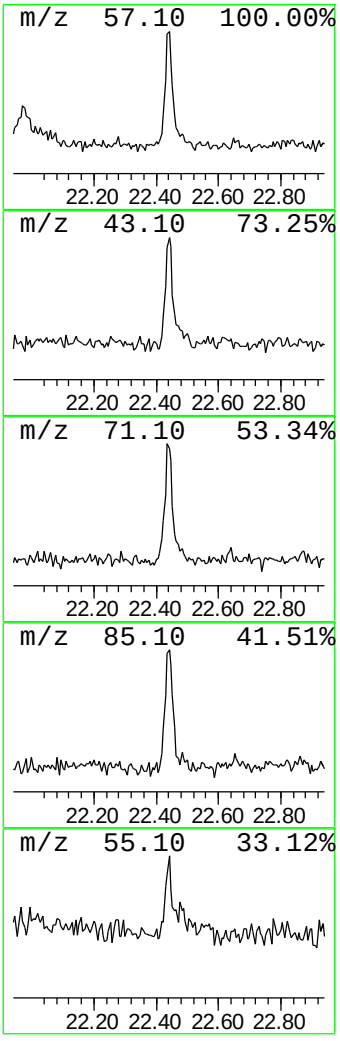
Peak Number 9 Bacchotricuneatin c Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.44	2.08 ng	81137	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	98
2	Nonadecane	268	C19H40	000629-92-5	92
3	Octadecane	254	C18H38	000593-45-3	89
4	Hexadecane	226	C16H34	000544-76-3	76
5	Hentriacontane	437	C31H64	000630-04-6	72





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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

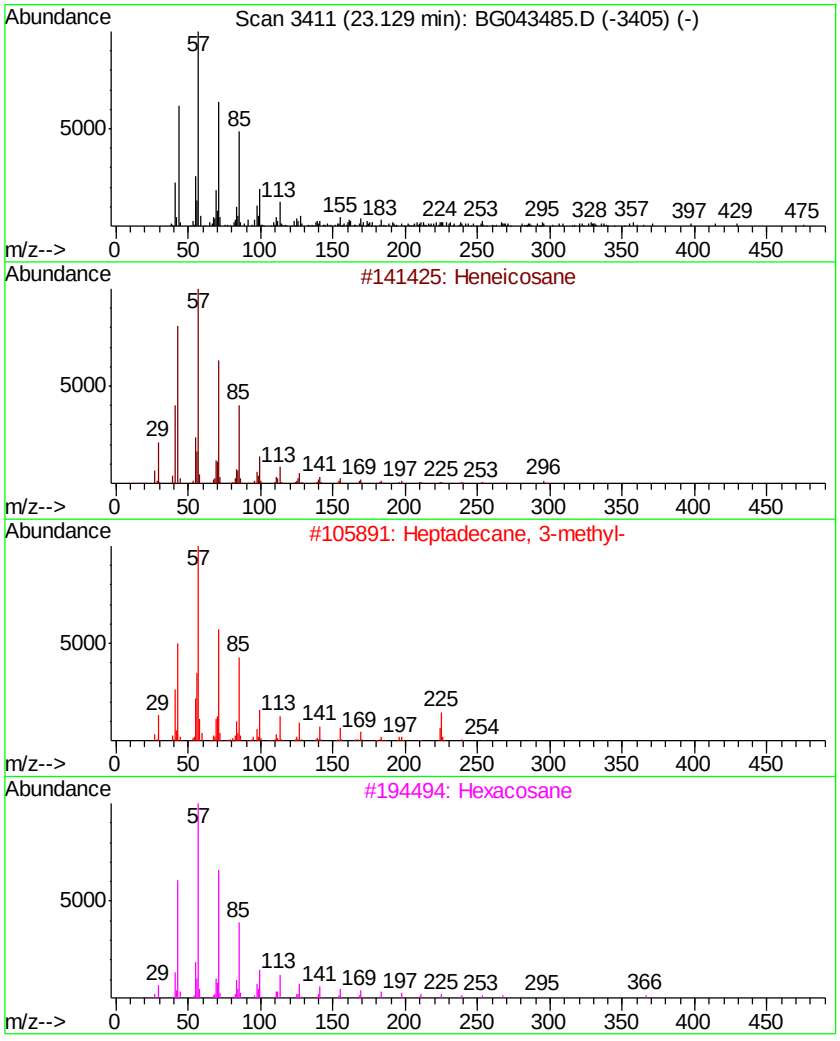
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

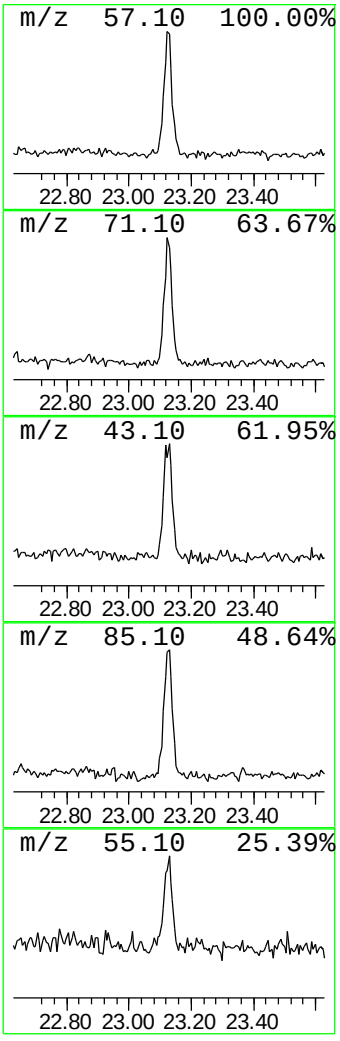
****

Peak Number 10 Heptadecane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.13	4.99 ng	194917	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	94
2	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	93
3	Hexacosane	366	C26H54	000630-01-3	87
4	Triacontane	422	C30H62	000638-68-6	87
5	Docosane	310	C22H46	000629-97-0	86





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Instrument : BNA_G
ClientSampleId : PAT-TOTE

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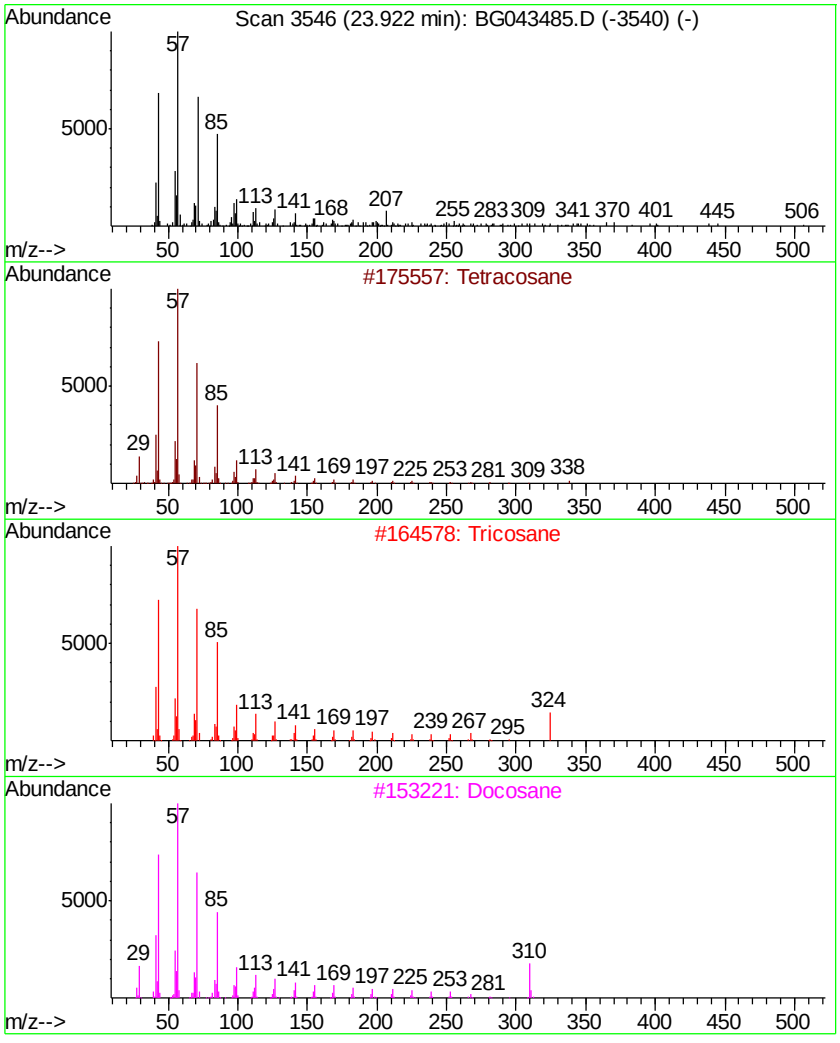
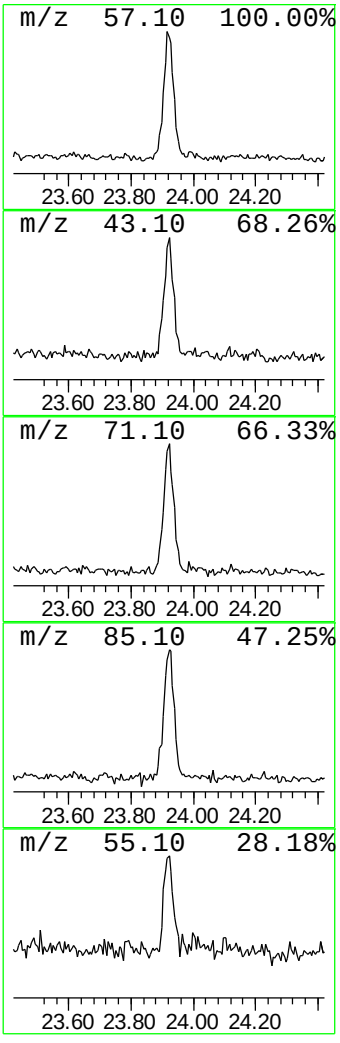
****

Peak Number 11 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	4.30 ng	240263	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	93
2	Tricosane	324	C23H48	000638-67-5	91
3	Docosane	310	C22H46	000629-97-0	91
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	90
5	Heneicosane	296	C21H44	000629-94-7	87





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Data File : BG043485.D
Acq On : 4 Nov 2019 17:50
Operator : JU
Sample : K5623-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAT-TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

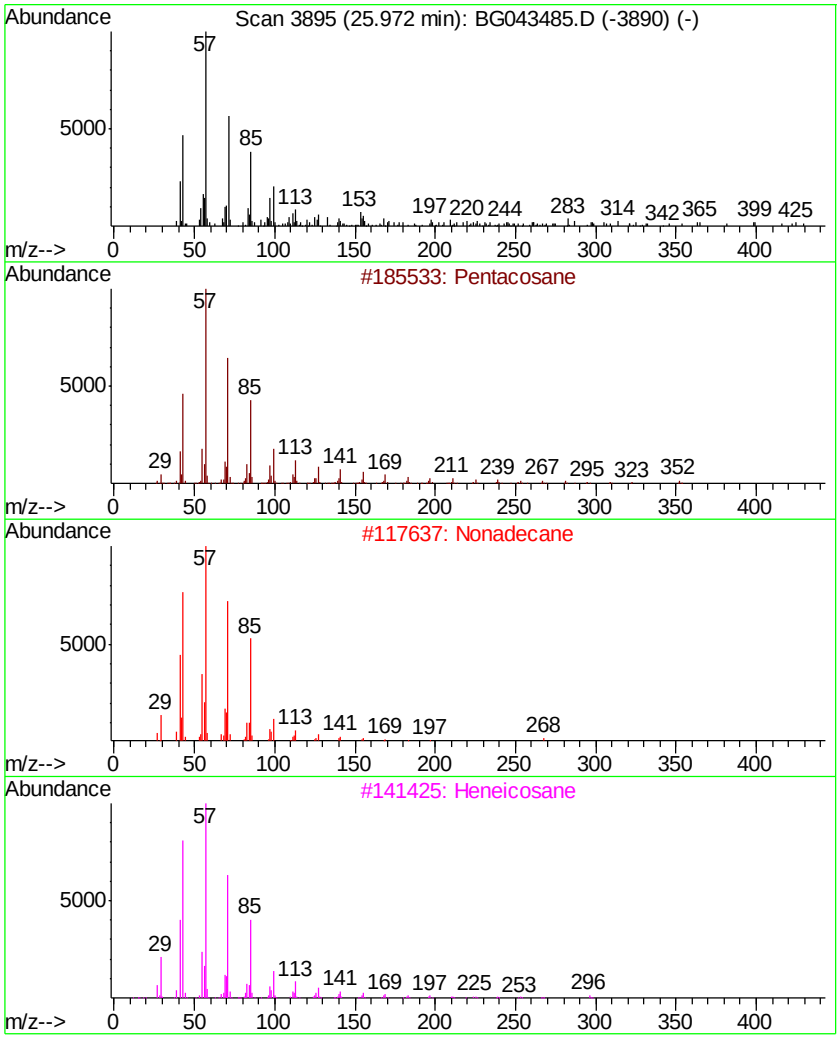
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

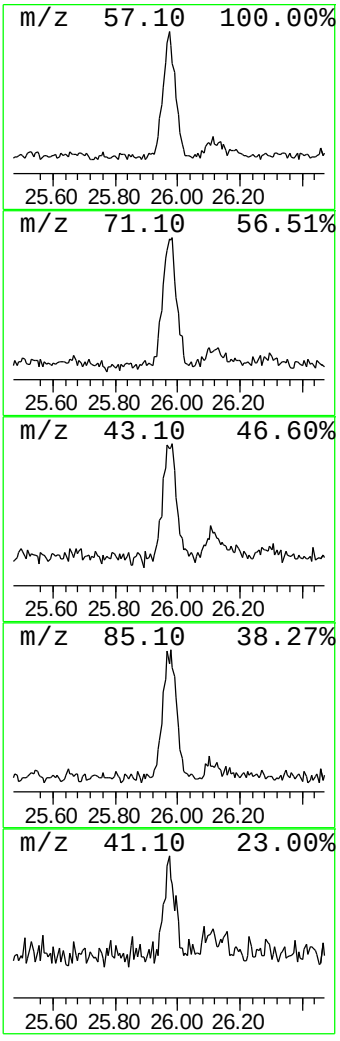
****

Peak Number 12 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.97	4.02 ng	224239	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Nonadecane	268	C19H40	000629-92-5	83
3	Heneicosane	296	C21H44	000629-94-7	64
4	Hexadecane	226	C16H34	000544-76-3	60
5	2-methyloctacosane	408	C29H60	1000376-72-8	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043485.D
Acq On : 4 Nov 2019 17:50
Operator : JU
Sample : K5623-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAT-TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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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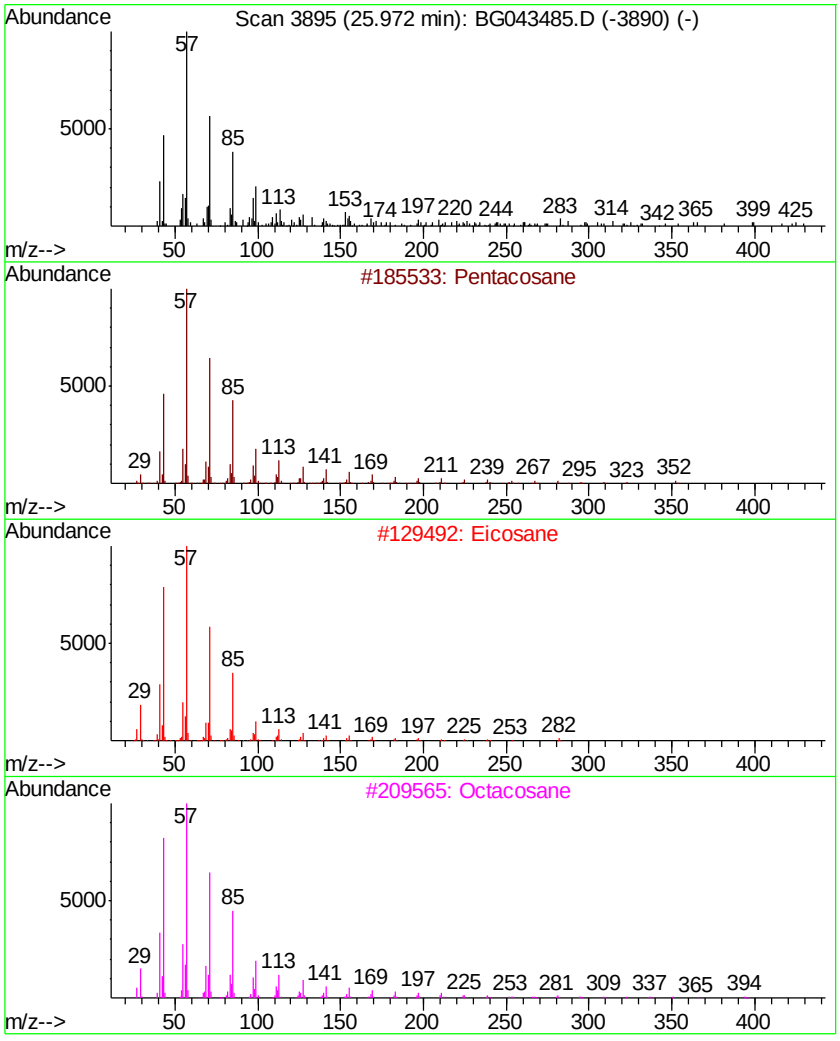
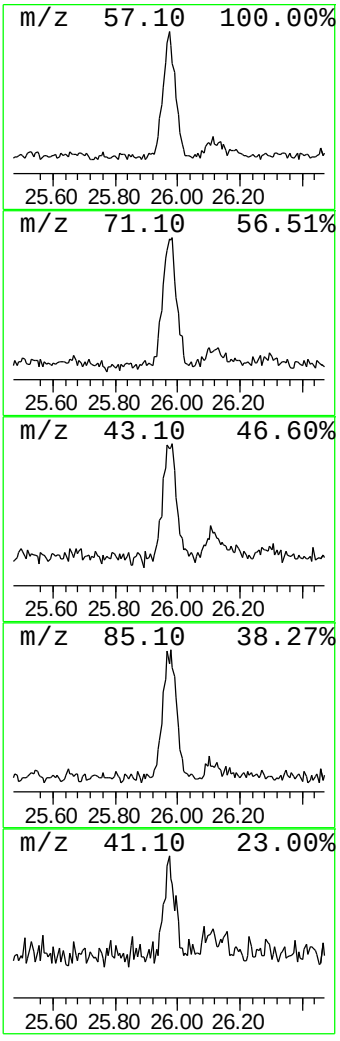
Peak Number 13 Pentacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.97	4.02 ng	224239	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	99
2	Eicosane	282	C20H42	000112-95-8	96
3	Octacosane	394	C28H58	000630-02-4	94
4	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	94
5	Hentriacontane	437	C31H64	000630-04-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110419\
Data File : BG043485.D
Acq On : 4 Nov 2019 17:50
Operator : JU
Sample : K5623-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAT-TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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...	3.18	88.2	ng	1321350	1	8.01	299686	20.0
2-Pentanone, 4-hy...	5.11	9.3	ng	138809	1	8.01	299686	20.0
unknown7.55	7.55	89.1	ng	1335540	1	8.01	299686	20.0
unknown11.58	11.58	27.1	ng	537008	2	10.82	396553	20.0
n-Hexadecanoic acid	18.29	27.4	ng	943948	4	17.39	689091	20.0
Octadecanoic acid	19.55	10.6	ng	413589	5	21.65	781355	20.0
1-Docosene	21.30	13.1	ng	513197	5	21.65	781355	20.0
Bacchotricuneatin c	22.44	2.1	ng	81137	5	21.65	781355	20.0
Heptadecane, 3-me...	23.13	5.0	ng	194917	5	21.65	781355	20.0
Tetracosane	23.92	4.3	ng	240263	6	24.85	1116480	20.0
Nonadecane	25.97	4.0	ng	224239	6	24.85	1116480	20.0
Pentacosane	25.97	4.0	ng	224239	6	24.85	1116480	20.0