LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110619\
Data File : BG043523.D
Acq On : 6 Nov 2019 16:56
Operator : JU
Sample : K5612-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GL-STOCKPILE

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	3.176	10	15	27	rVB	107521	194189	7.97%	1.450%
2	5.115	338	345	355	rBV	106914	176180	7.23%	1.315%
3	5.597	421	427	449	rBV	525532	921410	37.81%	6.879%
4	7.195	692	699	712	rBV	542820	1015309	41.66%	7.581%
5	7.554	751	760	771	rBV	586422	1035604	42.49%	7.732%
6	8.012	831	838	847	rBV	112138	194947	8.00%	1.456%
7	8.335	886	893	911	rBV	428358	765223	31.40%	5.713%
8	9.175	1025	1036	1053	rBV	279406	601575	24.68%	4.491%
9	10.820	1308	1316	1326	rBV	111024	240141	9.85%	1.793%
10	13.265	1723	1732	1746	rBV	785454	1376989	56.50%	10.281%
11	14.093	1867	1873	1885	rBV2	65835	128732	5.28%	0.961%
12	14.639	1960	1966	1978	rBV2	214052	381572	15.66%	2.849%
13	16.132	2212	2220	2243	rBV	686056	1304820	53.54%	9.742%
14	17.389	2426	2434	2449	rBV	260216	484713	19.89%	3.619%
15	17.507	2449	2454	2461	rVB3	24486	43077	1.77%	0.322%
16	18.276	2580	2585	2592	rBV5	28807	50628	2.08%	0.378%
17	19.998	2872	2878	2890	rBV	1810498	2437259	100.00%	18.197%
18	20.791	3009	3013	3017	rBV3	21542	27032	1.11%	0.202%
19	21.296	3095	3099	3114	rBV3	94356	235439	9.66%	1.758%
20	21.655	3154	3160	3172	rBV2	339119	713977	29.29%	5.331%
21	21.837	3188	3191	3196	rVB2	38022	58510	2.40%	0.437%
22	22.442	3290	3294	3299	rVB	45208	66470	2.73%	0.496%
23	23.124	3405	3410	3418	rVB	48566	88908	3.65%	0.664%
24	23.923	3540	3546	3554	rVB3	44950	98922	4.06%	0.739%
25	24.857	3694	3705	3719	rBV2	236206	752040	30.86%	5.615%

Sum of corrected areas: 13393666

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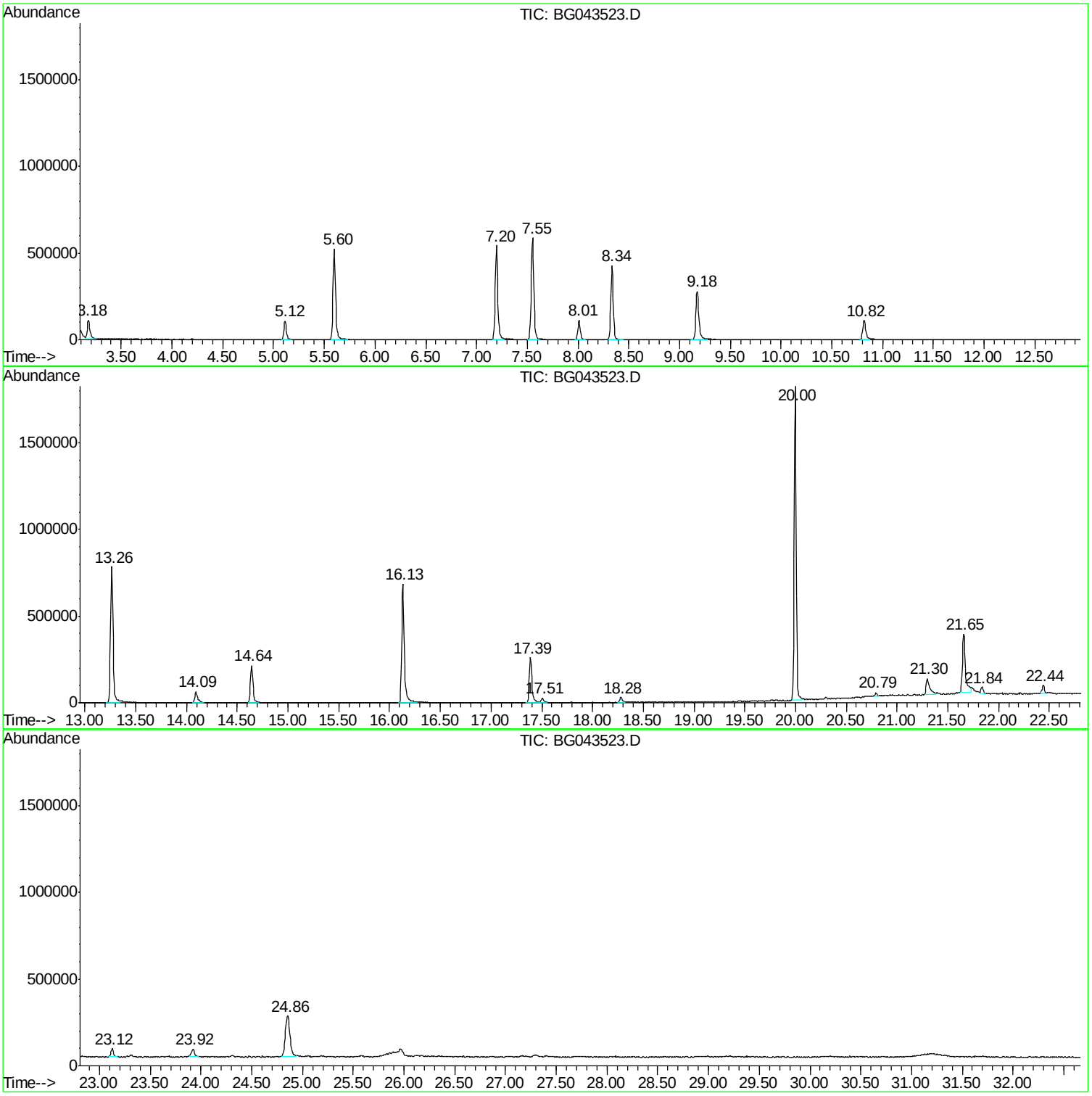
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GL-STOCKPILE

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110619\
Data File : BG043523.D
Acq On : 6 Nov 2019 16:56
Operator : JU
Sample : K5612-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GL-STOCKPILE

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

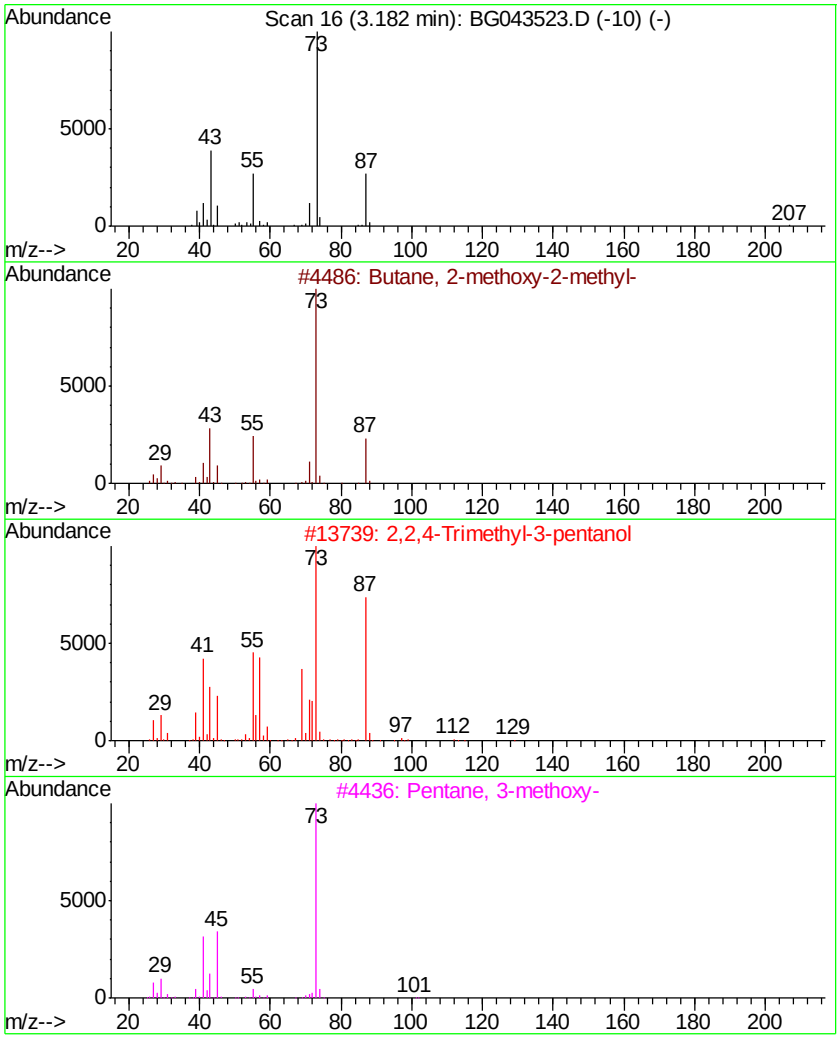
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

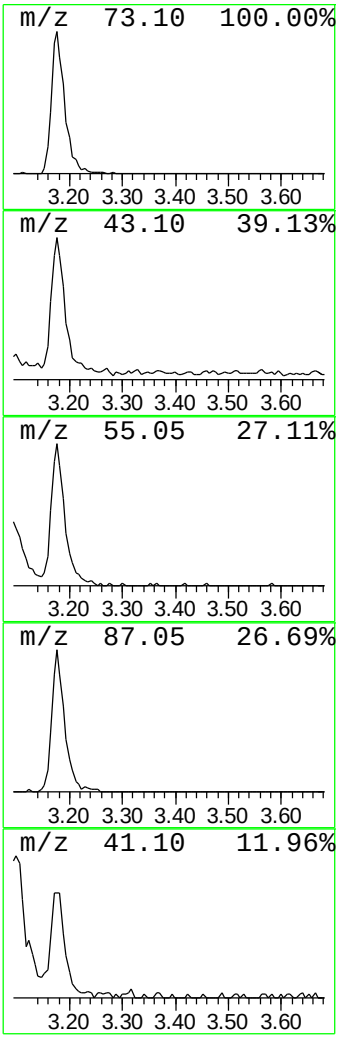
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	19.92 ng	194189	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	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9





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Data File : BG043523.D
Acq On : 6 Nov 2019 16:56
Operator : JU
Sample : K5612-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GL-STOCKPILE

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

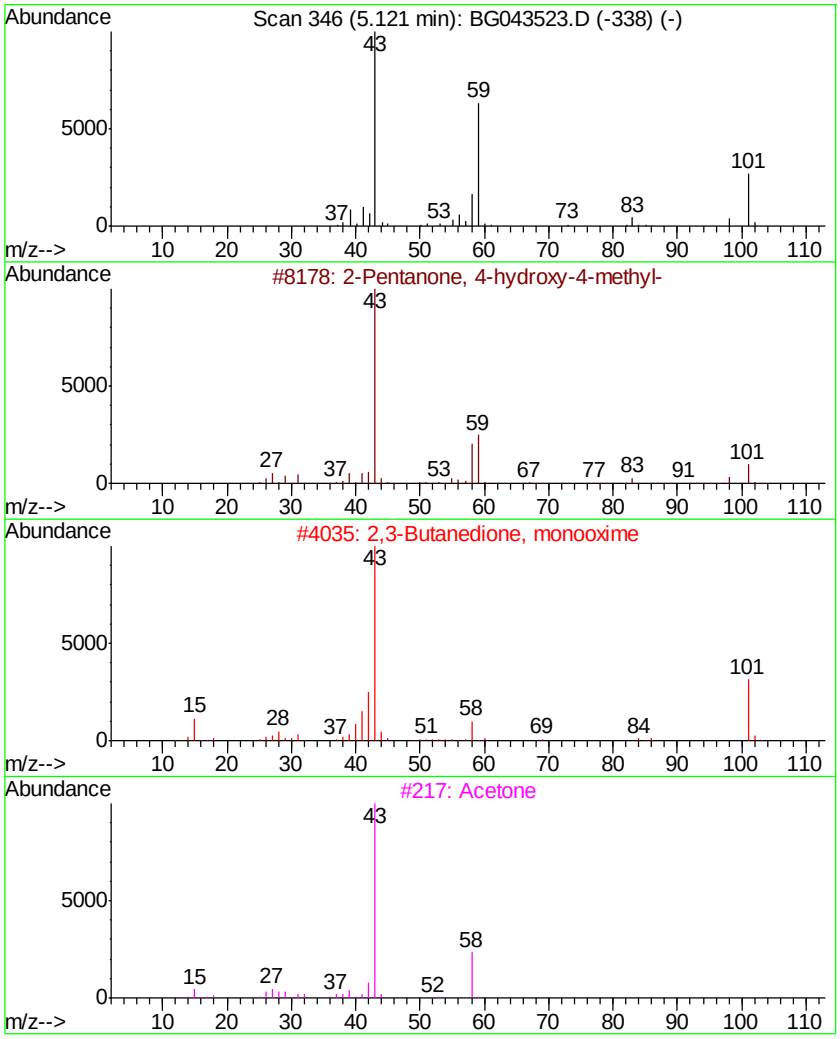
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

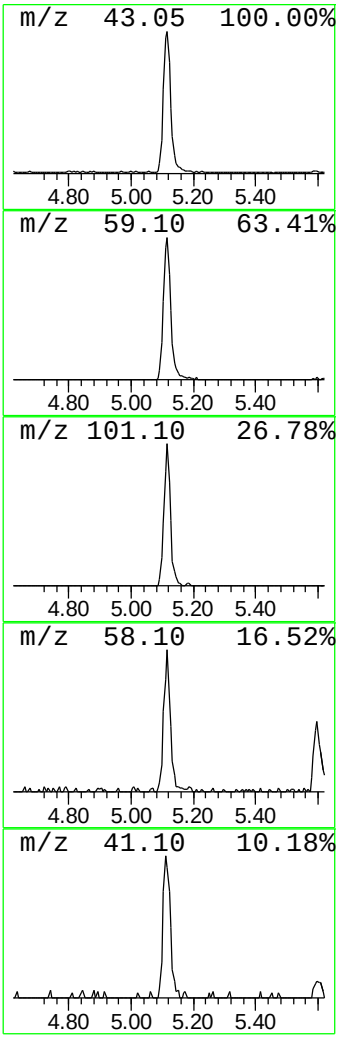
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	18.07 ng	176180	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	42
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Acetone	58	C3H6O	000067-64-1	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110619\
Data File : BG043523.D
Acq On : 6 Nov 2019 16:56
Operator : JU
Sample : K5612-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GL-STOCKPILE

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

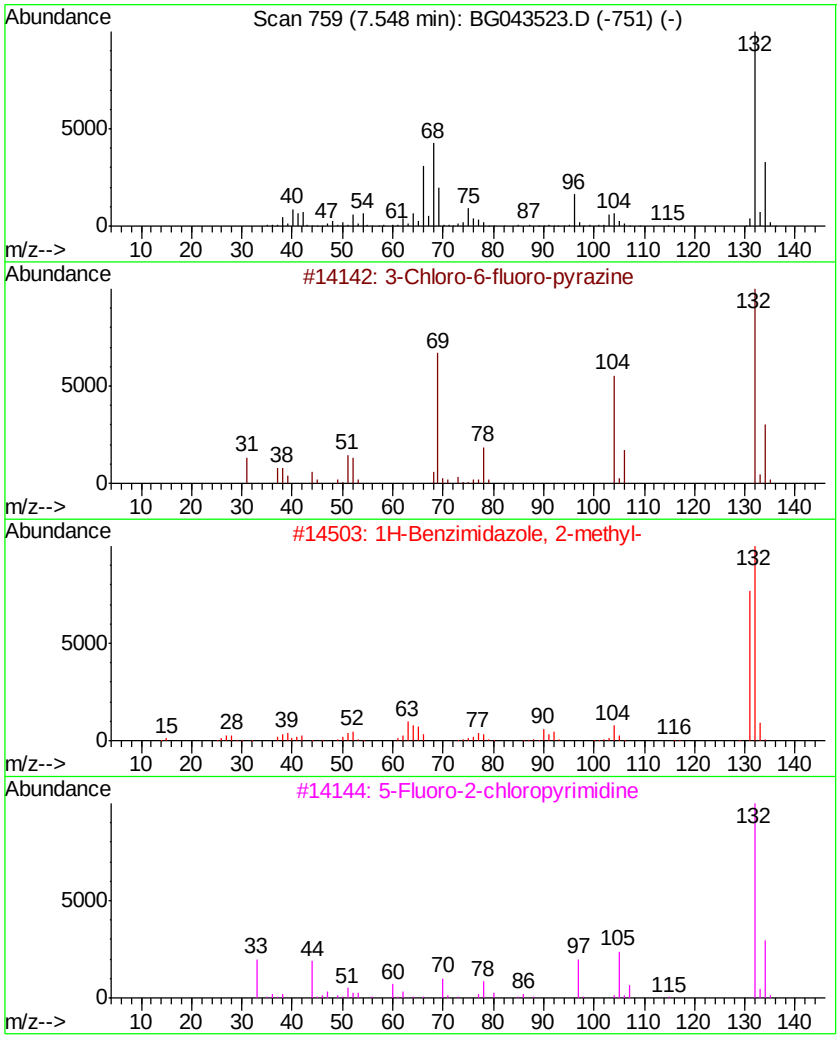
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

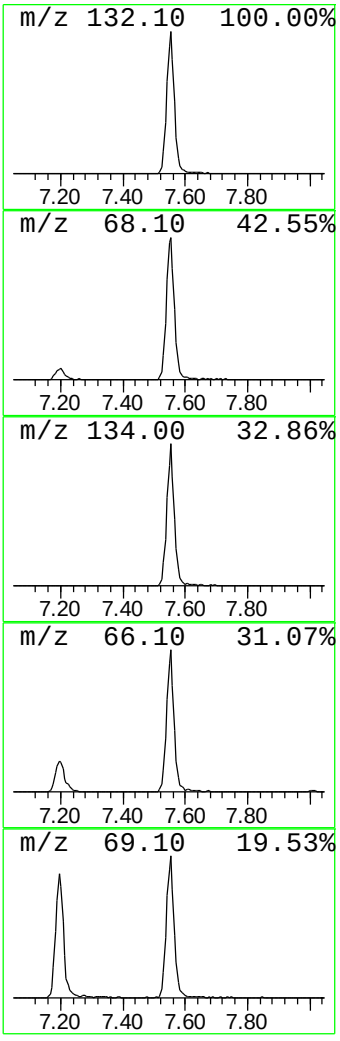
****

Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	106.25 ng	1035600	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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





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Acq On : 6 Nov 2019 16:56
Operator : JU
Sample : K5612-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GL-STOCKPILE

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

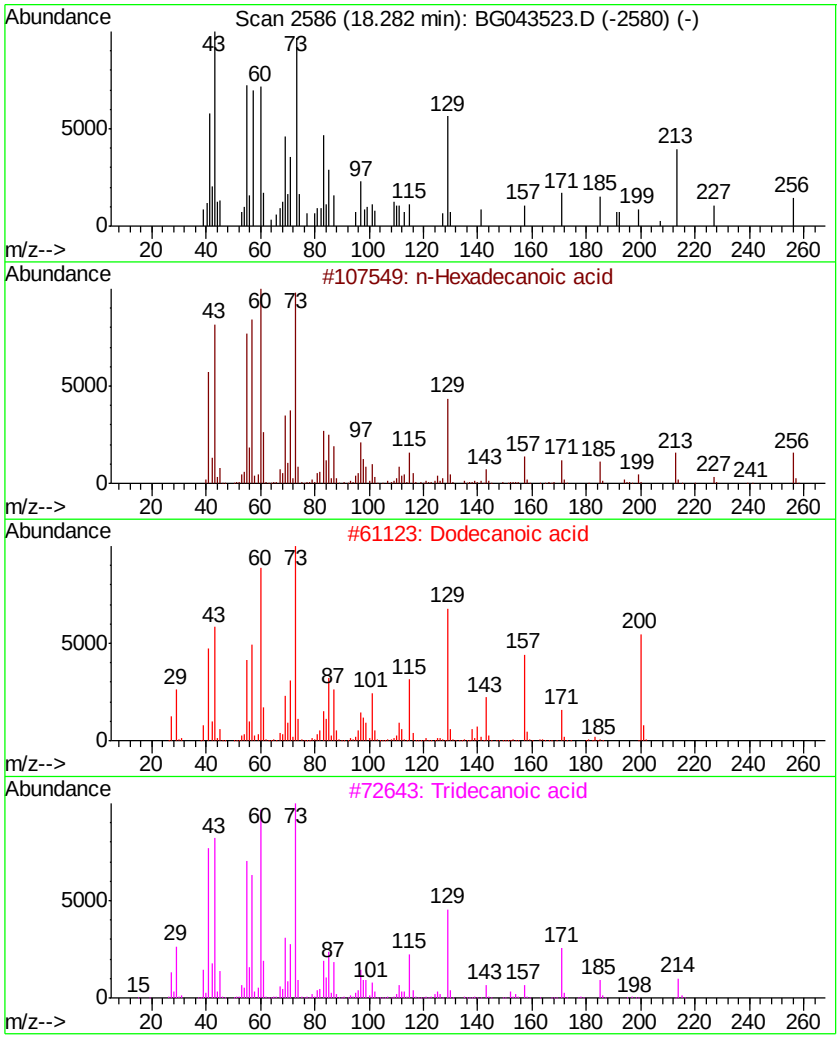
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

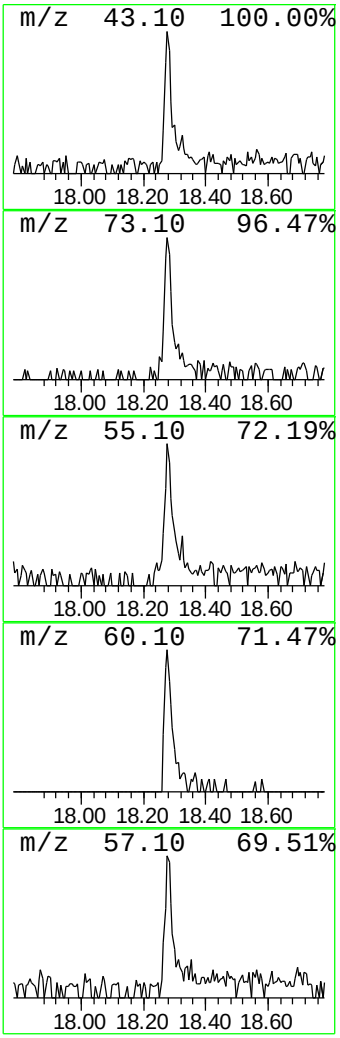
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	2.09 ng	50628	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Dodecanoic acid	200	C12H24O2	000143-07-7	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





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Sample : K5612-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GL-STOCKPILE

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

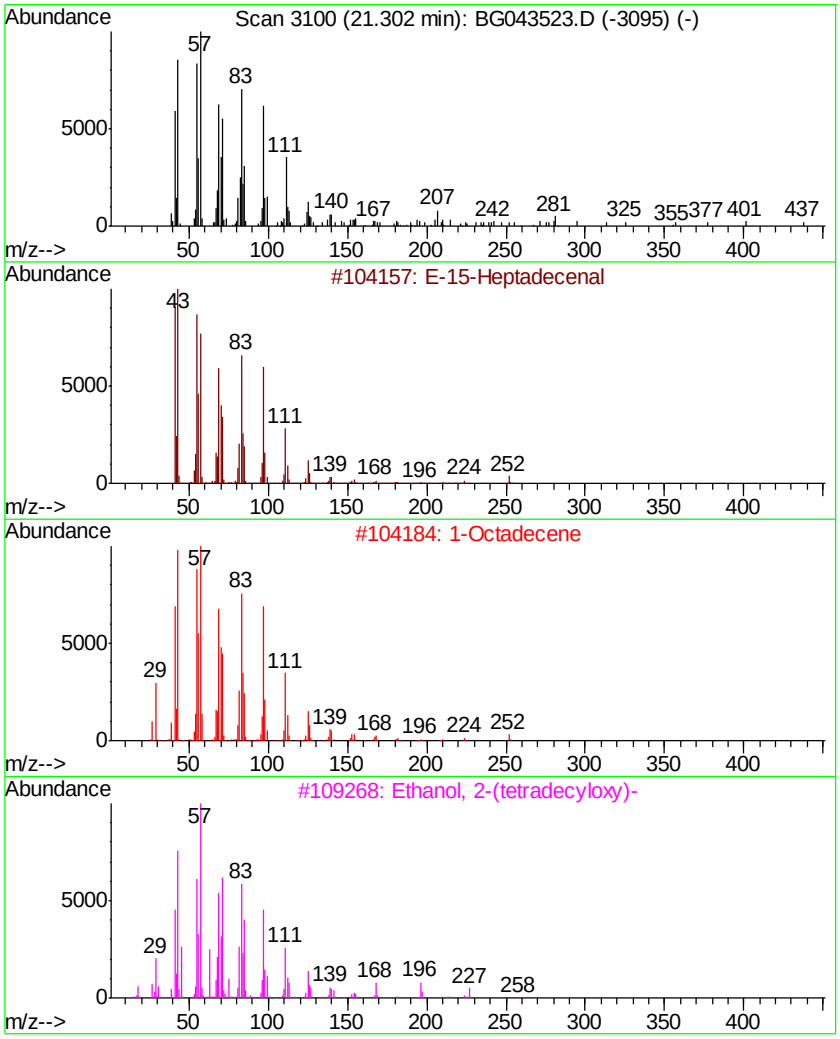
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

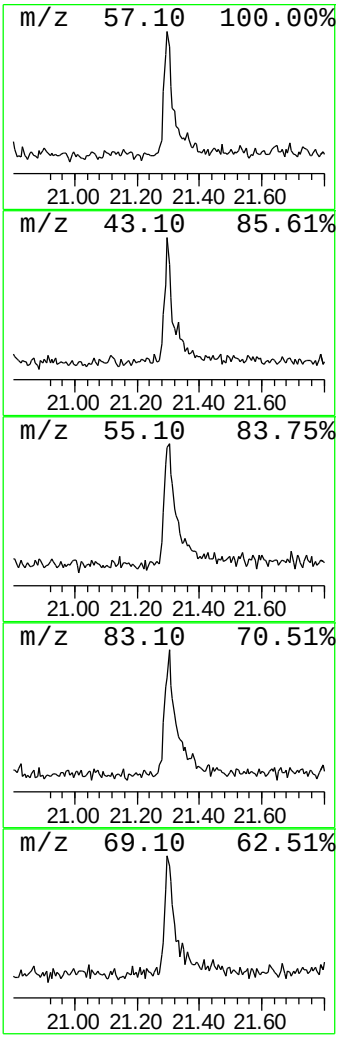
****

Peak Number 6 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	6.60 ng	235439	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
2	1-Octadecene	252	C18H36	000112-88-9	94
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87





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Data File : BG043523.D
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GL-STOCKPILE

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

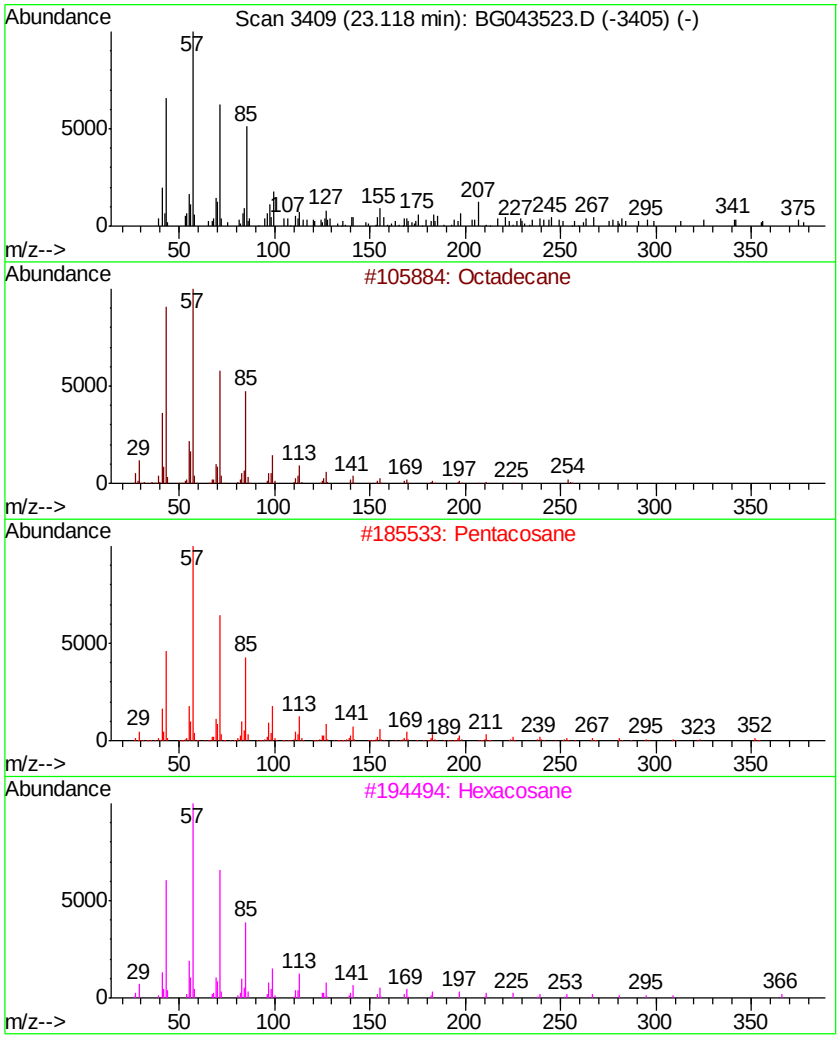
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

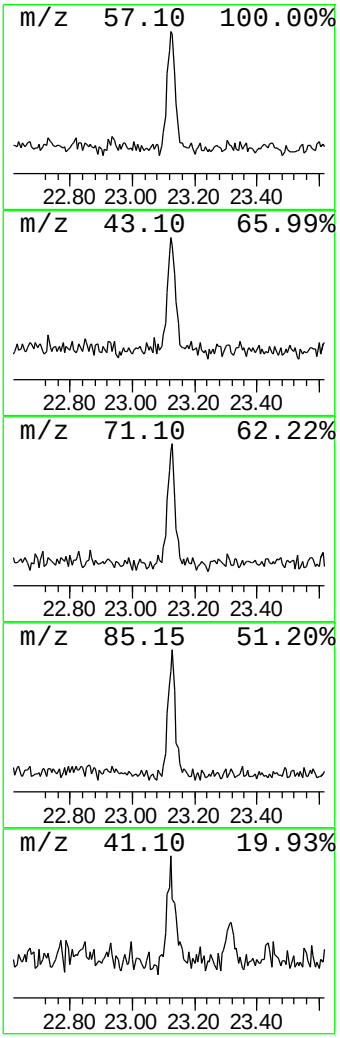
****

Peak Number 7 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.12	2.49 ng	88908	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	94
2	Pentacosane	352	C25H52	000629-99-2	93
3	Hexacosane	366	C26H54	000630-01-3	92
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	87
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	83





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Sample : K5612-04
Misc :
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Instrument : BNA_G
ClientSampleId : GL-STOCKPILE

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

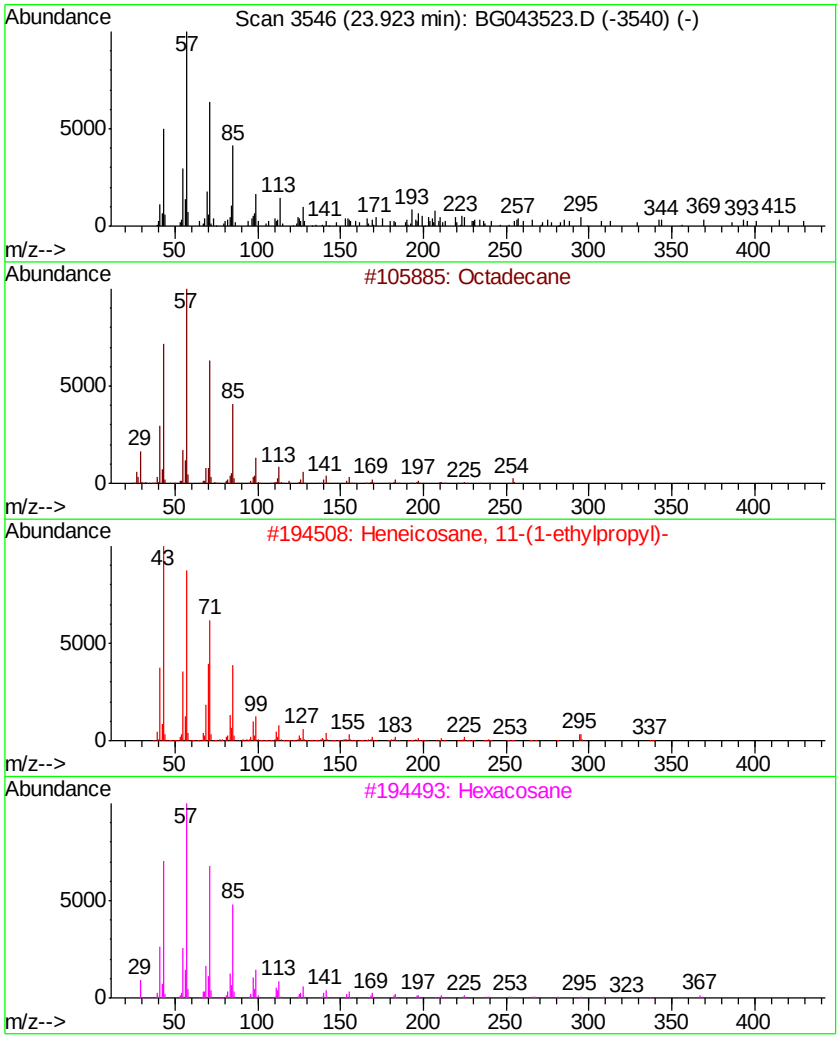
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

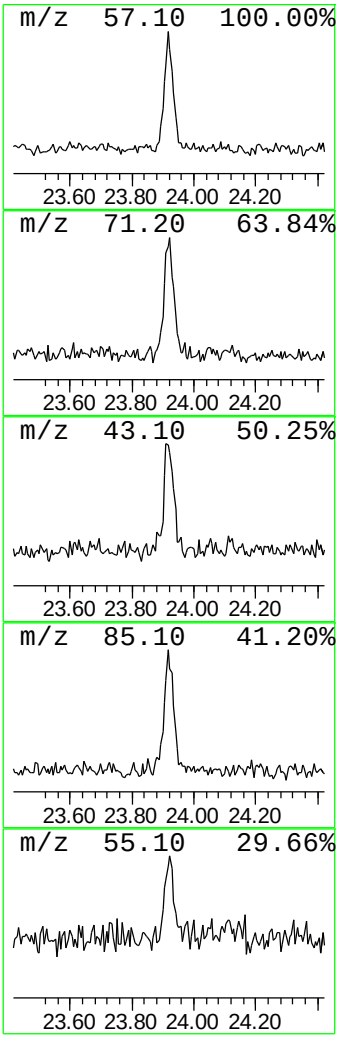
****

Peak Number 8 Heneicosane, 11-(1-ethylpro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	2.63 ng	98922	Perylene-d12	24.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	64
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	64
3	Hexacosane	366	C26H54	000630-01-3	64
4	Heptadecane	240	C17H36	000629-78-7	64
5	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	64





Tentatively Identified Compound (LSC) summary

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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	19.9	ng	194189	1	8.01	194947	20.0
2-Pentanone, 4-hy...	5.12	18.1	ng	176180	1	8.01	194947	20.0
unknown7.55	7.55	106.3	ng	1035600	1	8.01	194947	20.0
n-Hexadecanoic acid	18.28	2.1	ng	50628	4	17.39	484713	20.0
E-15-Heptadecenal	21.30	6.6	ng	235439	5	21.65	713977	20.0
Octadecane	23.12	2.5	ng	88908	5	21.65	713977	20.0
Heneicosane, 11-(...	23.92	2.6	ng	98922	6	24.86	752040	20.0