LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001025.D
Acq On : 11 Nov 2019 19:41
Operator : JU
Sample : K5763-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-34-D

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_P\METHODS\8270-BP110619.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	2.122	3	6	12	rVB2	157617	272674	3.71%	0.490%
2	2.346	38	44	55	rVB	569961	881698	12.01%	1.586%
3	5.740	617	621	634	rBV	472992	706489	9.62%	1.271%
4	6.310	711	718	722	rBV	3329272	4053909	55.21%	7.291%
5	7.816	966	974	985	rBV	3451445	4628270	63.03%	8.324%
6	8.010	998	1007	1012	rBV	3771336	4667241	63.56%	8.394%
7	8.375	1063	1069	1074	rBV	1290852	1506222	20.51%	2.709%
8	8.616	1104	1110	1114	rBV	3258234	3903614	53.16%	7.021%
9	9.245	1210	1217	1221	rBV	2316725	2825199	38.47%	5.081%
10	10.398	1407	1413	1418	rBV	1640463	1892845	25.78%	3.404%
11	12.180	1707	1716	1720	rBV	5123697	6287162	85.62%	11.308%
12	12.845	1824	1829	1835	rVB	330111	383348	5.22%	0.689%
13	13.263	1893	1900	1905	rBV	1872547	2338394	31.85%	4.206%
14	14.551	2112	2119	2133	rBV	3377231	4181712	56.95%	7.521%
15	15.651	2301	2306	2311	rBV	2170254	2537511	34.56%	4.564%
16	16.539	2452	2457	2470	rBV2	276305	424343	5.78%	0.763%
17	17.621	2638	2641	2651	rBV	108983	155368	2.12%	0.279%
18	17.933	2688	2694	2698	rBV	6670372	7342973	100.00%	13.207%
19	19.157	2898	2902	2911	rBV2	552274	701162	9.55%	1.261%
20	19.292	2920	2925	2929	rBV	2261841	2529497	34.45%	4.549%
21	19.321	2929	2930	2938	rVB2	63786	87172	1.19%	0.157%
22	19.974	3038	3041	3048	rVB	94291	106650	1.45%	0.192%
23	20.351	3103	3105	3110	rVB	78998	82127	1.12%	0.148%
24	20.439	3115	3120	3124	rVB	401079	488381	6.65%	0.878%
25	20.756	3170	3174	3183	rBV	78866	153260	2.09%	0.276%
26	21.074	3222	3228	3235	rVB	1794572	2463322	33.55%	4.430%

Sum of corrected areas: 55600543

LSC Report - Integrated Chromatogram

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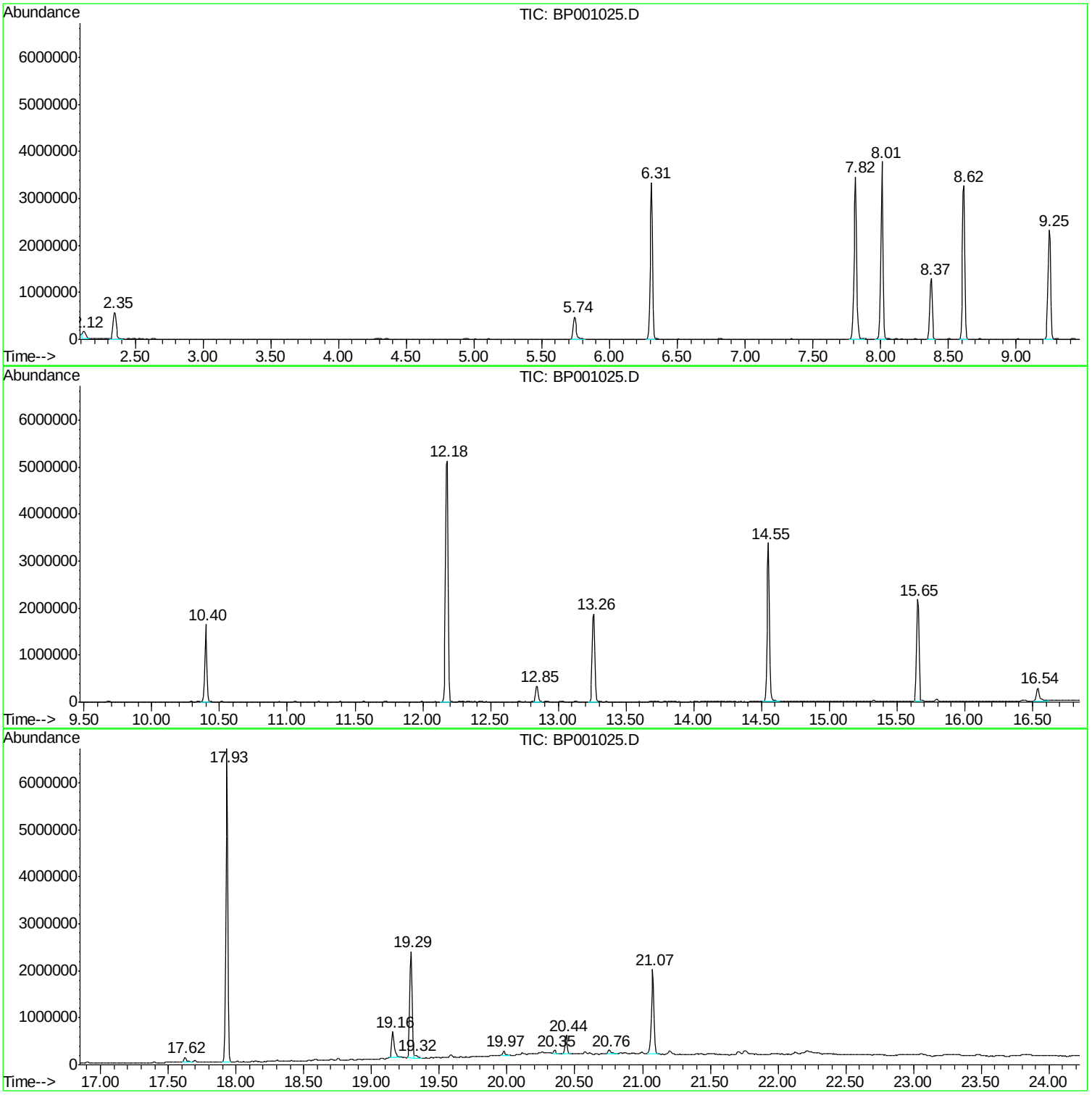
Data File : BP001025.D
Acq On : 11 Nov 2019 19:41
Operator : JU
Sample : K5763-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-34-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

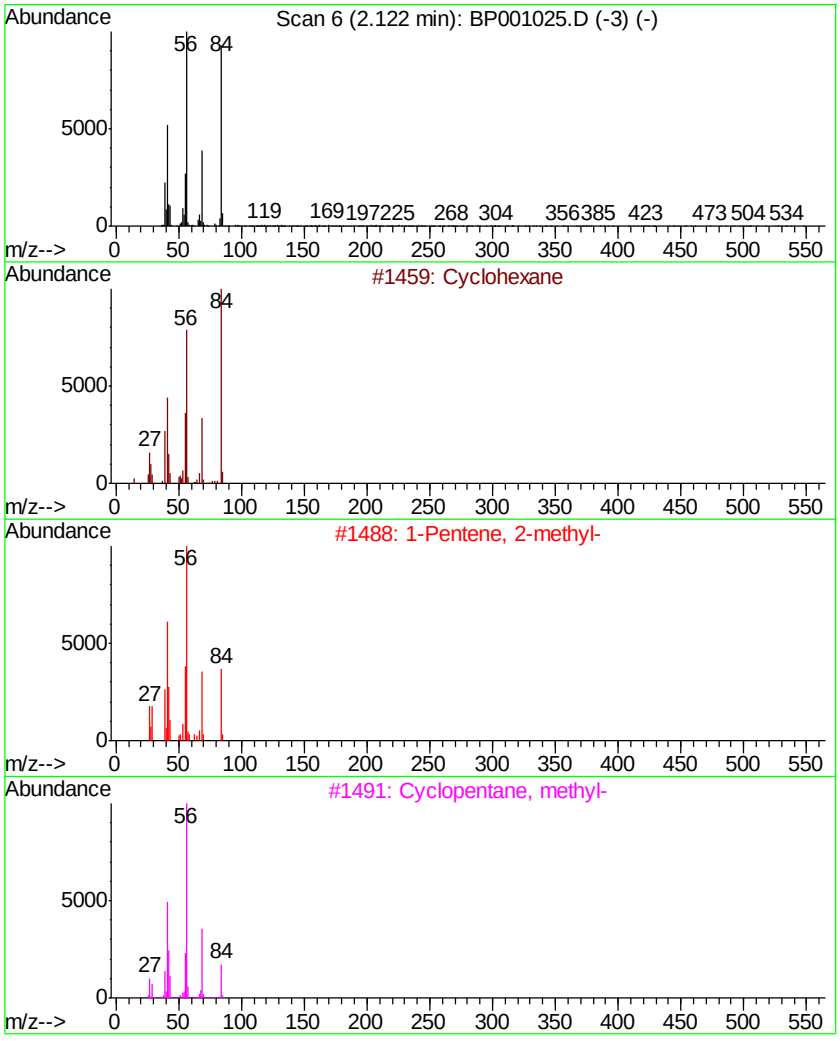
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

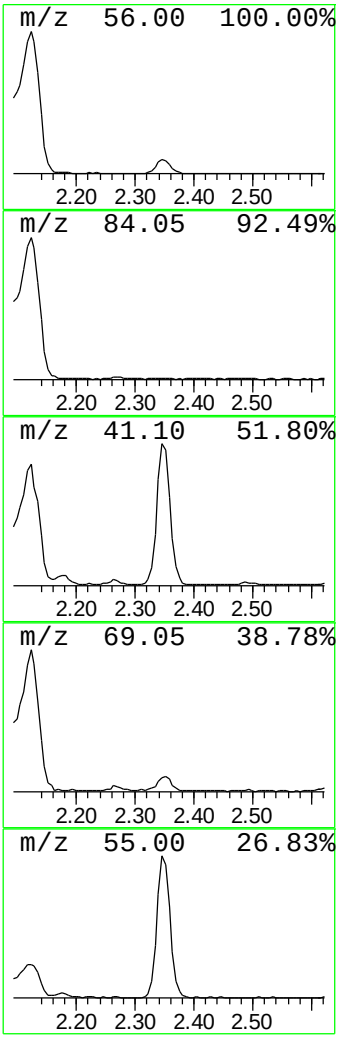
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	3.62 ng	272674	1,4-Dichlorobenzene-d4	8.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	80
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	56
4	2-Acetylpiperidine	127	C7H13NO	097073-22-8	56
5	Iron pentacarbonyl	196	C5FeO5	013463-40-6	56





Library Search Compound Report

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Data File : BP001025.D
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Sample : K5763-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-34-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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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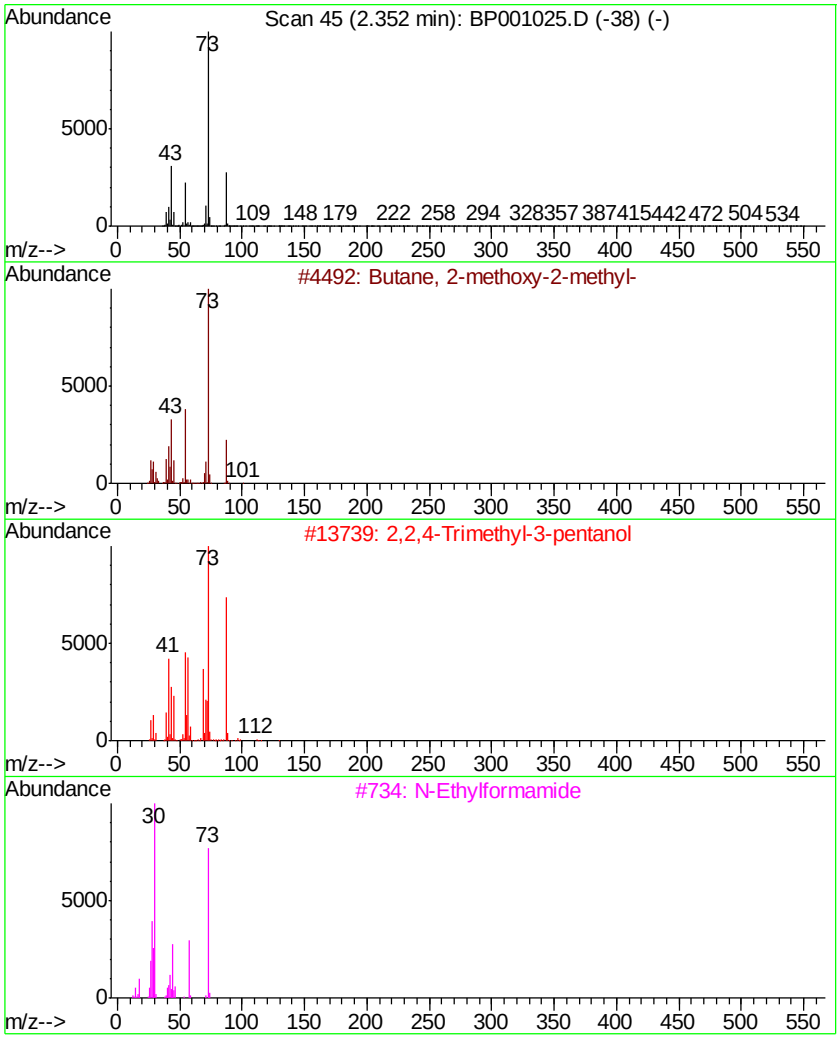
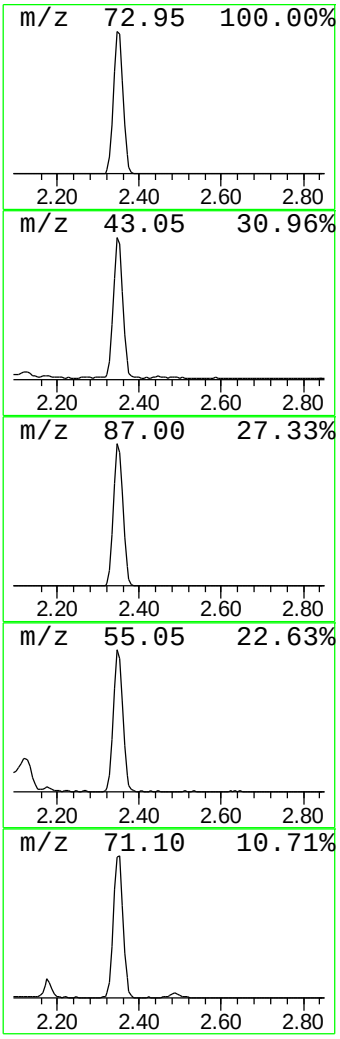
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	11.71 ng	881698	1,4-Dichlorobenzene-d4	8.37

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	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

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Data File : BP001025.D
Acq On : 11 Nov 2019 19:41
Operator : JU
Sample : K5763-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-34-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

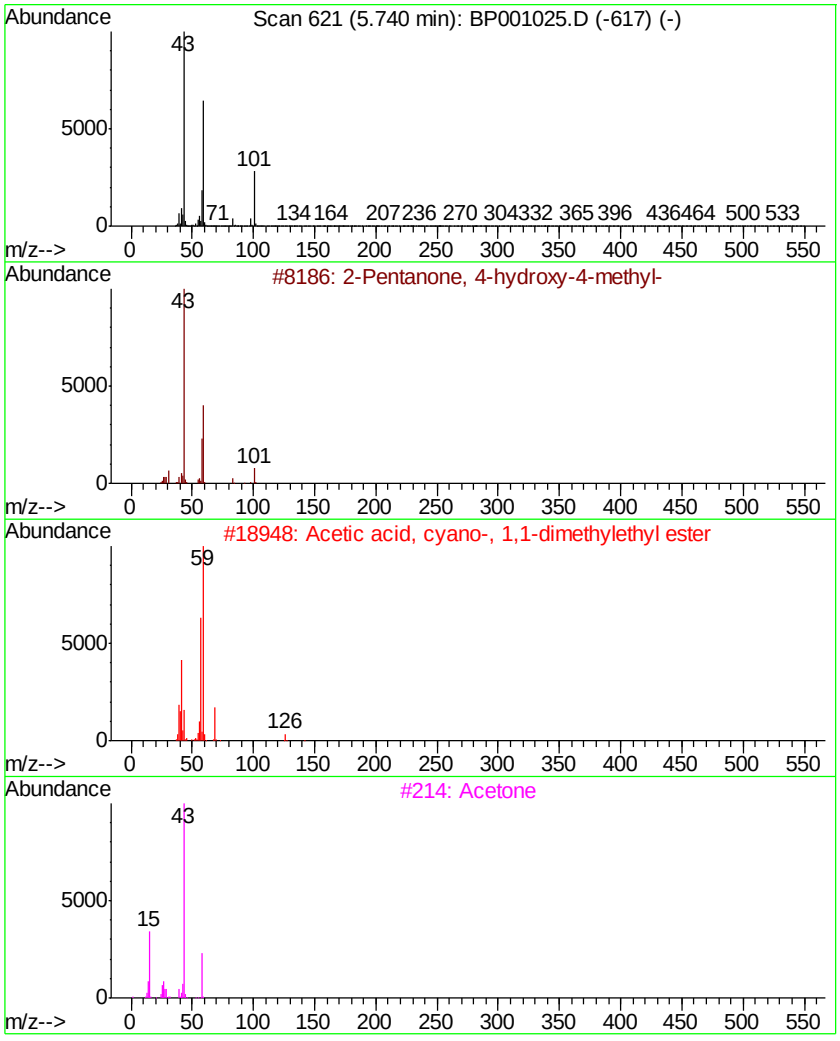
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

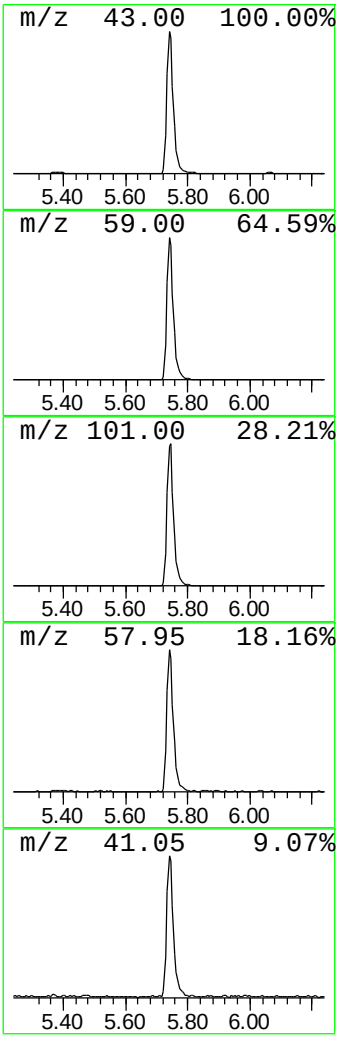
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.74	9.38 ng	706489	1,4-Dichlorobenzene-d4	8.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
3	Acetone	58	C3H6O	000067-64-1	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Operator : JU
Sample : K5763-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-34-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

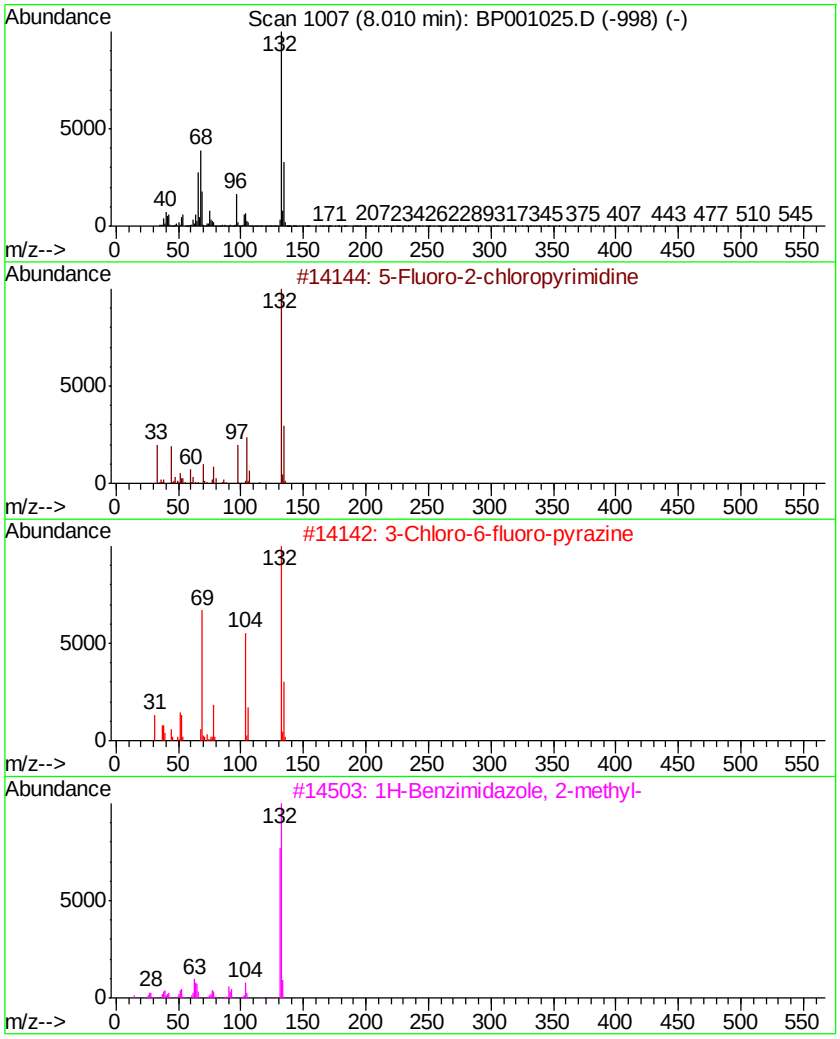
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

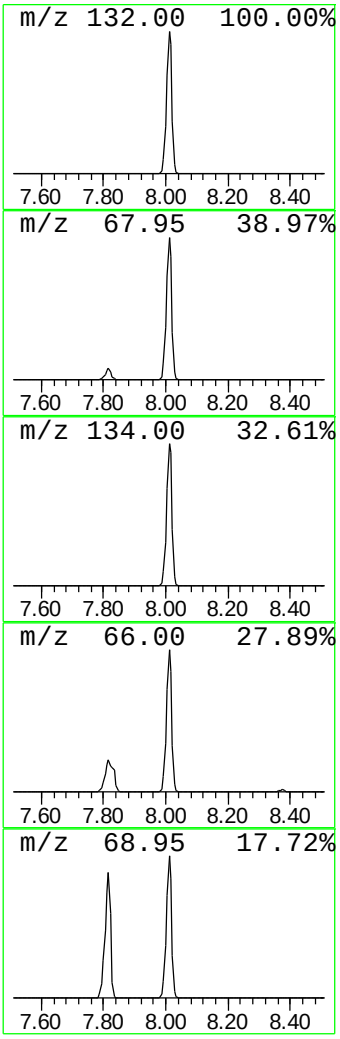
****

Peak Number 4 unknown8.01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	61.97 ng	4667240	1,4-Dichlorobenzene-d4	8.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10





Library Search Compound Report

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Instrument : BNA_P
ClientSampleId : TP-34-D

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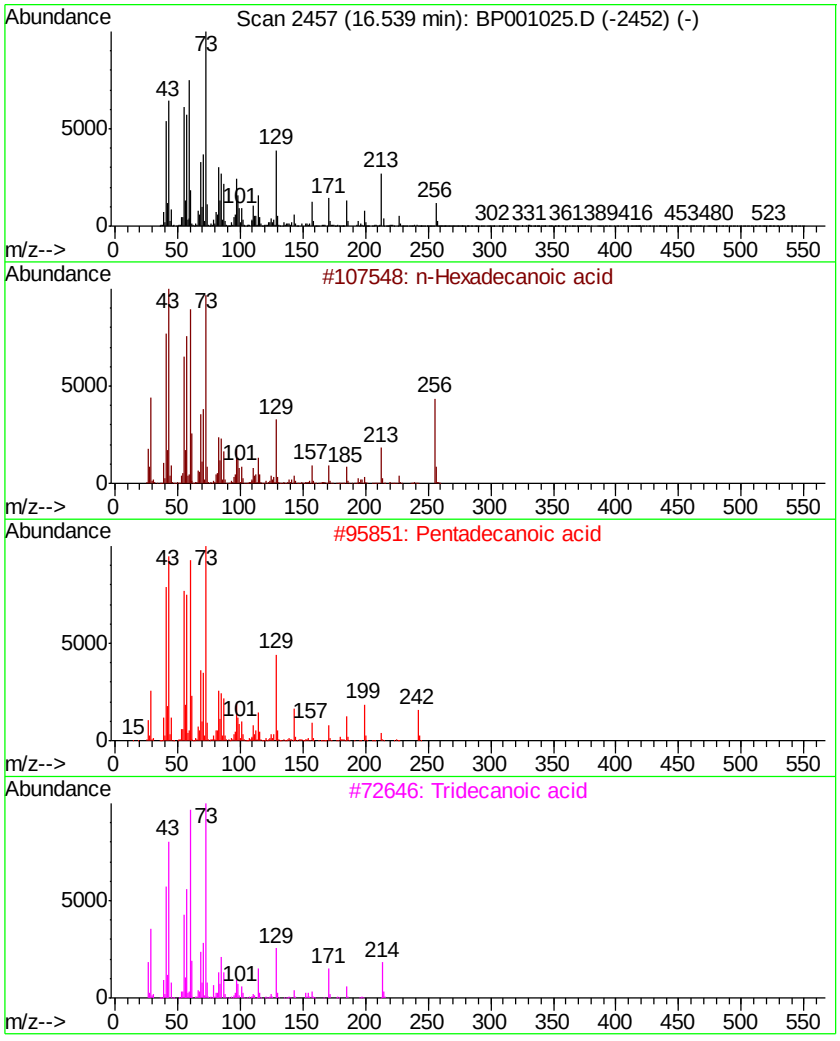
TIC Integration Parameters: LSCINT.P

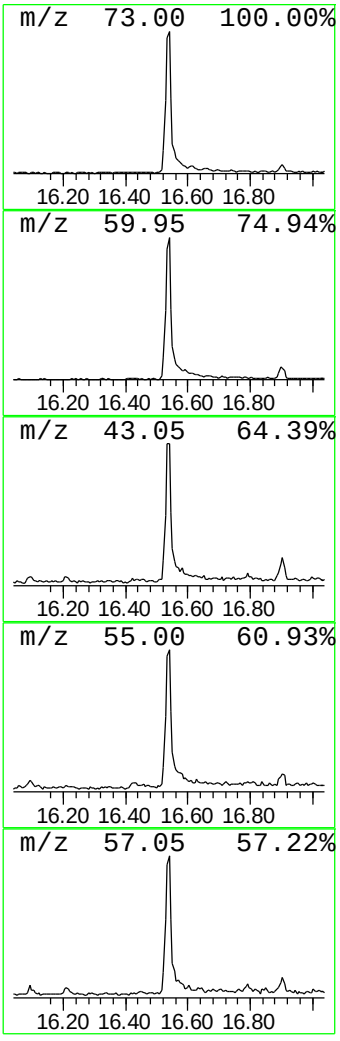
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	3.34 ng	424343	Phenanthrene-d10	15.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Octadecanoic acid	284	C18H36O2	000057-11-4	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Library Search Compound Report

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Instrument : BNA_P
ClientSampleId : TP-34-D

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

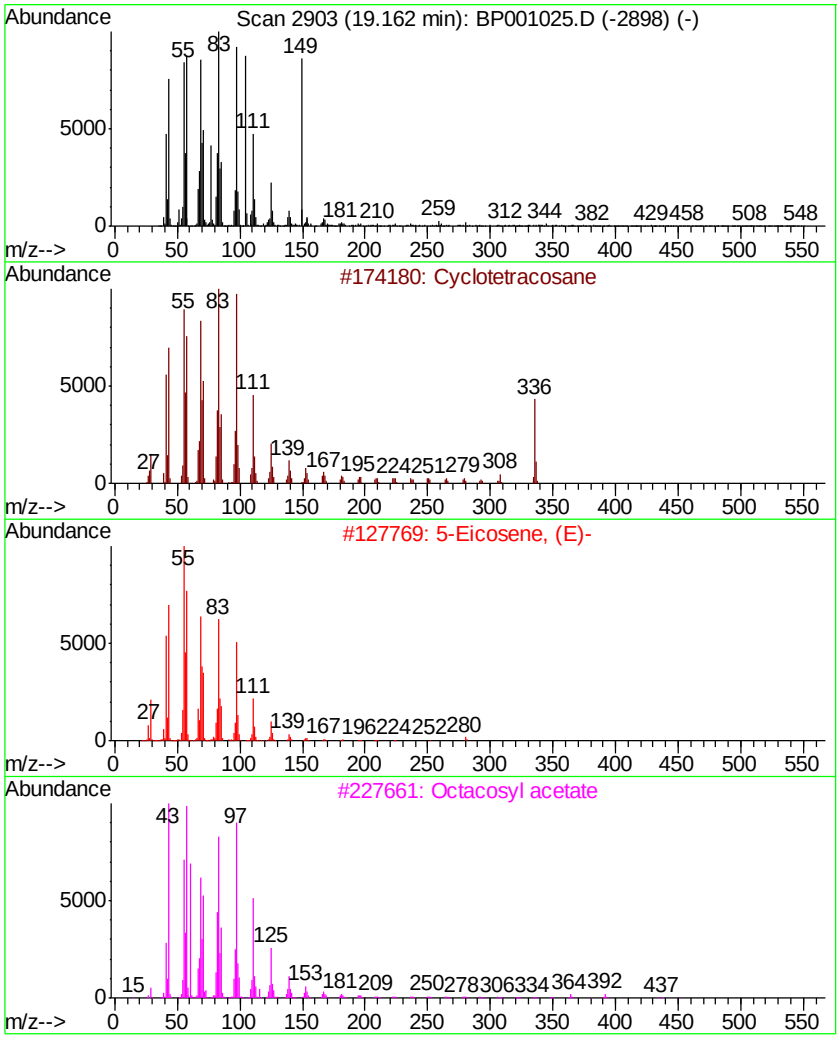
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

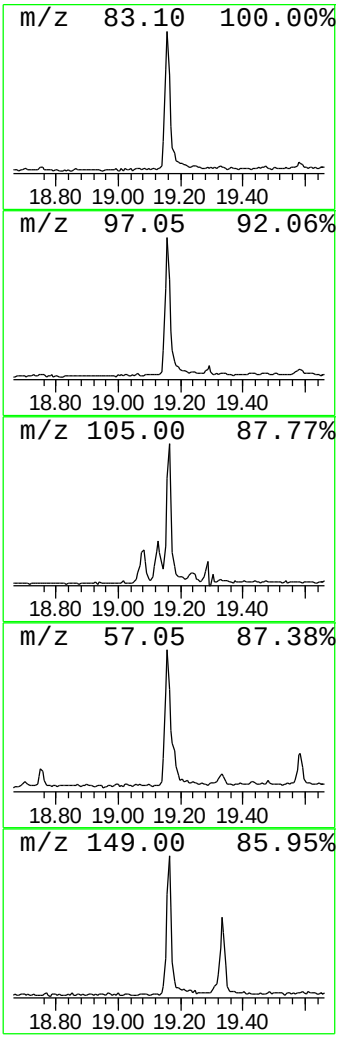
****

Peak Number 7 Cyclotetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.16	5.54 ng	701162	Chrysene-d12	19.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	99
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
3	Octacosyl acetate	452	C30H60O2	018206-97-8	96
4	Cyclopentadecane	210	C15H30	000295-48-7	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

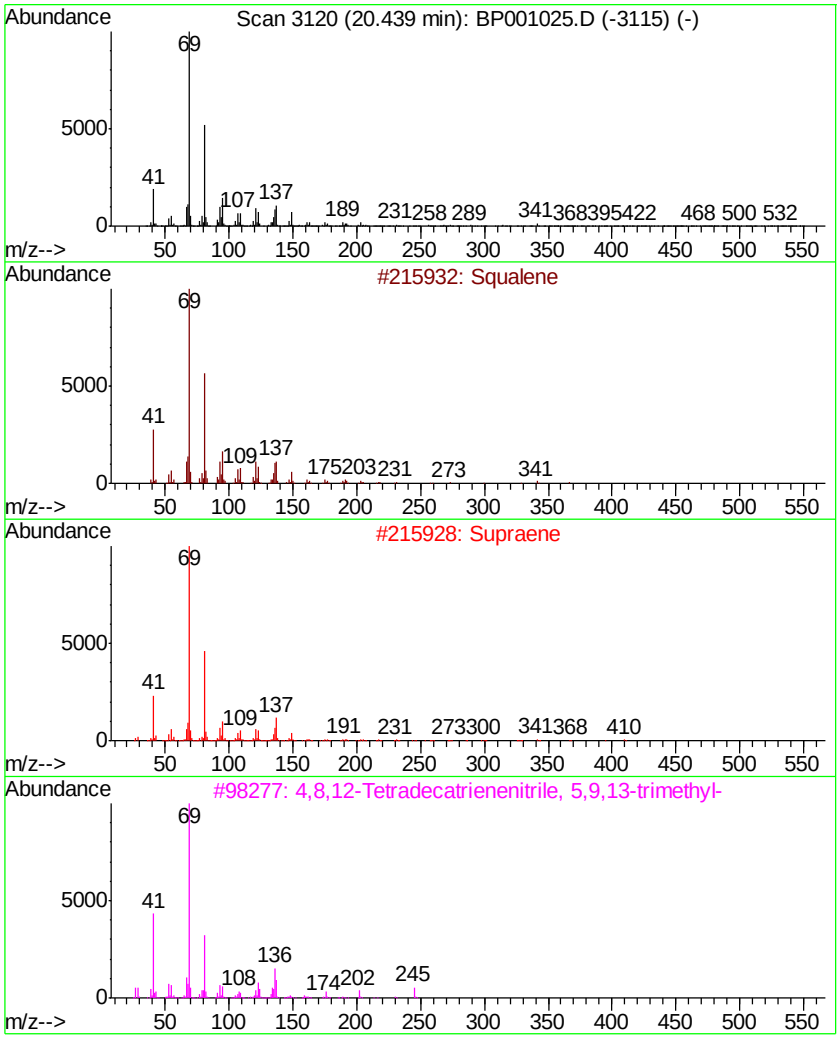
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

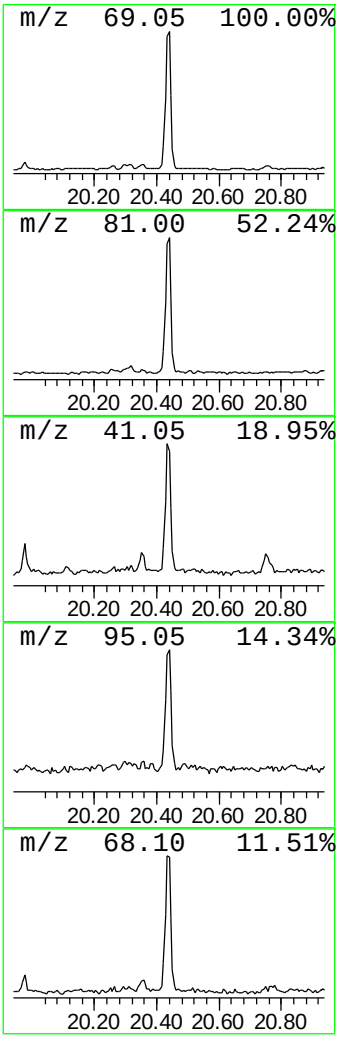
****

Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.44	3.97 ng	488381	Perylene-d12	21.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	94
2	Supraene	410	C30H50	007683-64-9	91
3	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50





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
1-Pentene, 2-methyl-	2.12	3.6	ng	272674	1	8.37	1506220	20.0
Butane, 2-methoxy...	2.35	11.7	ng	881698	1	8.37	1506220	20.0
2-Pentanone, 4-hy...	5.74	9.4	ng	706489	1	8.37	1506220	20.0
unknown8.01	8.01	62.0	ng	4667240	1	8.37	1506220	20.0
n-Hexadecanoic acid	16.54	3.3	ng	424343	4	15.65	2537510	20.0
Cyclotetracosane	19.16	5.5	ng	701162	5	19.29	2529500	20.0
Squalene	20.44	4.0	ng	488381	6	21.07	2463320	20.0