LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080718\
Data File : BM016239.D
Acq On : 08 Aug 2018 04:44
Operator : SJ/JU
Sample : J4310-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-3

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_M\METHODS\8270-BM072318.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	5.181	318	322	331	rBV	81530	128937	4.98%	0.720%
2	5.663	398	404	423	rBV	563894	949685	36.69%	5.305%
3	7.304	676	683	701	rBV	635906	1083091	41.85%	6.050%
4	7.663	737	744	757	rBV	709097	1157801	44.74%	6.467%
5	8.133	818	824	836	rBB	213472	348782	13.48%	1.948%
6	8.457	872	879	891	rBB	525289	850952	32.88%	4.753%
7	9.051	975	980	992	rBV2	12939	26739	1.03%	0.149%
8	9.322	1019	1026	1037	rBV	391741	661277	25.55%	3.694%
9	10.951	1297	1303	1310	rBV	273749	449331	17.36%	2.510%
10	13.392	1711	1718	1727	rBV	992044	1415164	54.68%	7.905%
11	14.227	1853	1860	1868	rVB	54875	78744	3.04%	0.440%
12	14.774	1944	1953	1959	rBV2	358111	553256	21.38%	3.090%
13	16.256	2200	2205	2216	rBV	855800	1206826	46.63%	6.741%
14	17.509	2412	2418	2421	rBV	486152	693236	26.79%	3.872%
15	17.551	2421	2425	2432	rVB	234132	339890	13.13%	1.898%
16	17.639	2436	2440	2446	rBV	41857	59937	2.32%	0.335%
17	17.921	2480	2488	2491	rBV3	22477	42168	1.63%	0.236%
18	18.356	2557	2562	2569	rBV2	132301	236606	9.14%	1.322%
19	18.421	2569	2573	2579	rVB	71342	106758	4.12%	0.596%
20	18.503	2581	2587	2590	rBV	19100	26766	1.03%	0.150%
21	18.568	2592	2598	2601	rBV2	44399	85039	3.29%	0.475%
22	18.603	2601	2604	2607	rVB	26810	30833	1.19%	0.172%
23	18.862	2644	2648	2653	rVV	36829	47738	1.84%	0.267%
24	18.927	2654	2659	2665	rVB3	32014	49769	1.92%	0.278%
25	19.103	2682	2689	2692	rBV6	18123	33112	1.28%	0.185%
26	19.274	2712	2718	2723	rBV3	39117	76396	2.95%	0.427%
27	19.339	2723	2729	2731	rBV5	18941	34051	1.32%	0.190%
28	19.433	2737	2745	2749	rBV5	27948	55350	2.14%	0.309%
29	19.539	2758	2763	2769	rVB	408206	561368	21.69%	3.136%
30	19.615	2769	2776	2786	rVB7	46760	101784	3.93%	0.569%
31	19.868	2814	2819	2821	rBV2	75816	115196	4.45%	0.643%
32	19.903	2821	2825	2832	rVV	345385	473939	18.31%	2.647%
33	19.968	2832	2836	2842	rVB2	32883	47059	1.82%	0.263%
34	20.086	2851	2856	2861	rBV	2227622	2588098	100.00%	14.456%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080718\
Data File : BM016239.D
Acq On : 08 Aug 2018 04:44
Operator : SJ/JU
Sample : J4310-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-3

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_M\METHODS\8270-BM072318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.215	2873	2878	2885	rBV5	34088	85822	3.32%	0.479%
36	20.292	2887	2891	2894	rBV4	23926	30994	1.20%	0.173%
37	20.356	2899	2902	2904	rVV3	51722	67668	2.61%	0.378%
38	20.386	2905	2907	2912	rVB2	50958	63100	2.44%	0.352%
39	20.486	2921	2924	2927	rBV3	25017	29669	1.15%	0.166%
40	20.680	2954	2957	2961	rBV	30713	46267	1.79%	0.258%
41	21.133	3030	3034	3039	rBV	56705	83946	3.24%	0.469%
42	21.309	3061	3064	3070	rVB3	112296	190801	7.37%	1.066%
43	21.638	3113	3120	3123	rBV2	717780	1146852	44.31%	6.406%
44	21.674	3123	3126	3131	rVB	203202	240624	9.30%	1.344%
45	23.268	3394	3397	3402	rBV	91407	163949	6.33%	0.916%
46	23.774	3479	3483	3489	rVB2	115008	203103	7.85%	1.134%
47	23.874	3496	3500	3508	rVB2	115907	219373	8.48%	1.225%
48	23.974	3512	3517	3524	rVV2	321135	615387	23.78%	3.437%

Sum of corrected areas: 17903233

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Instrument : BNA_M
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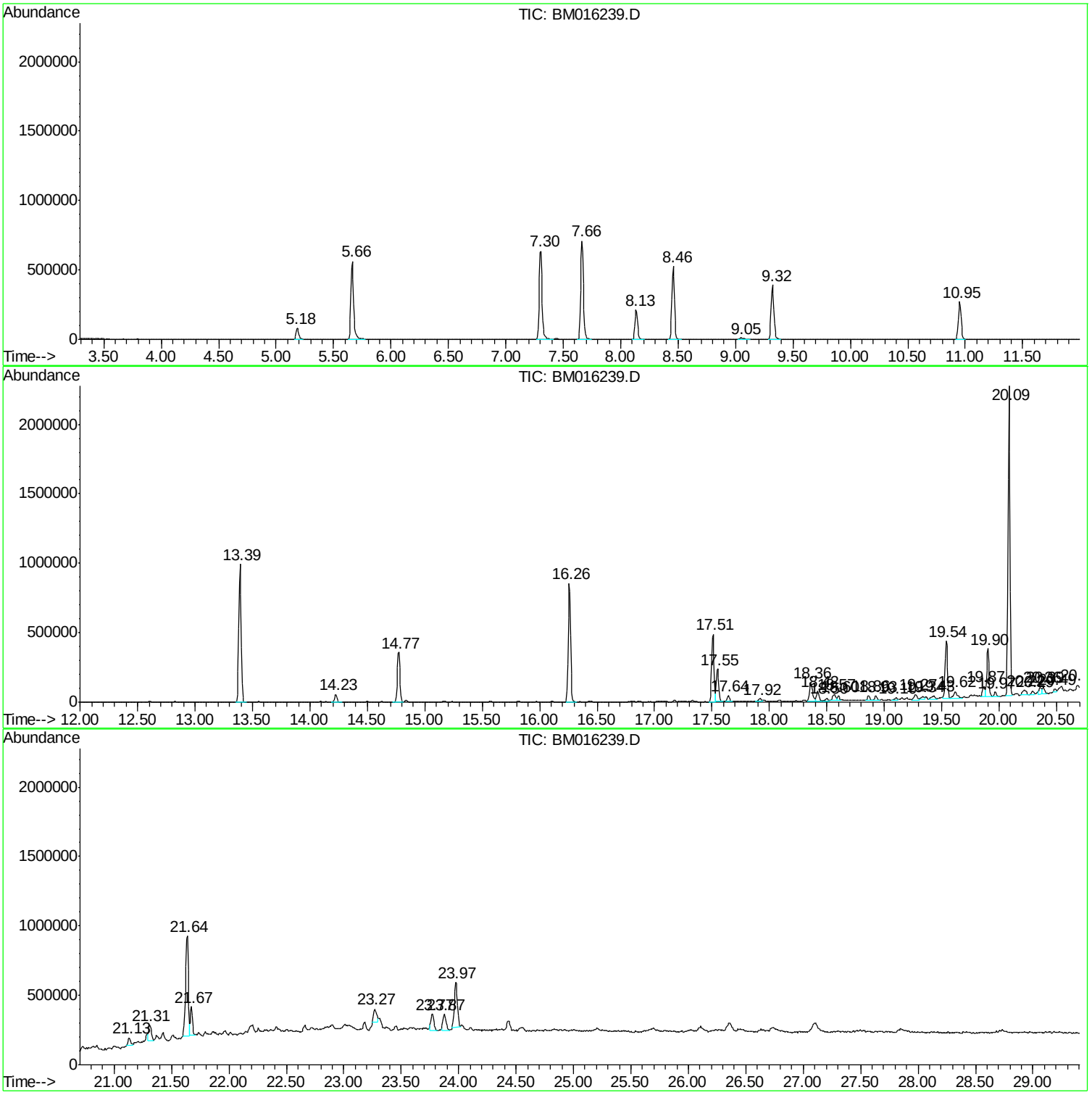
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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

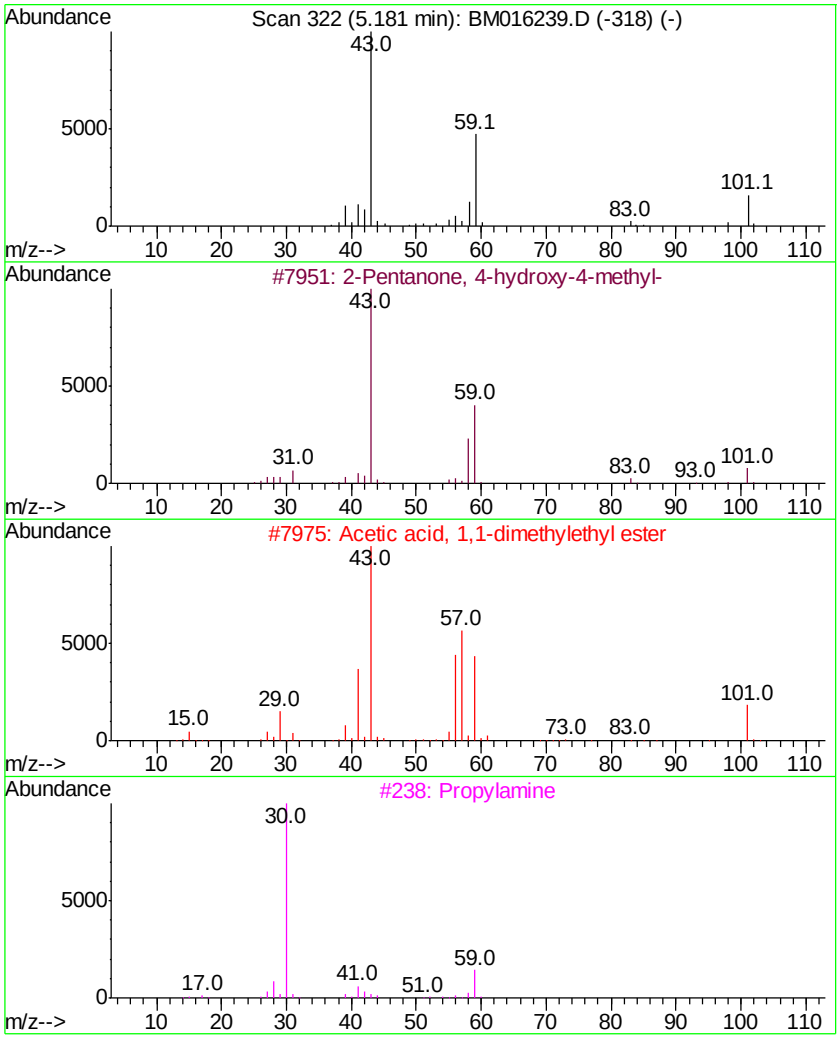
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

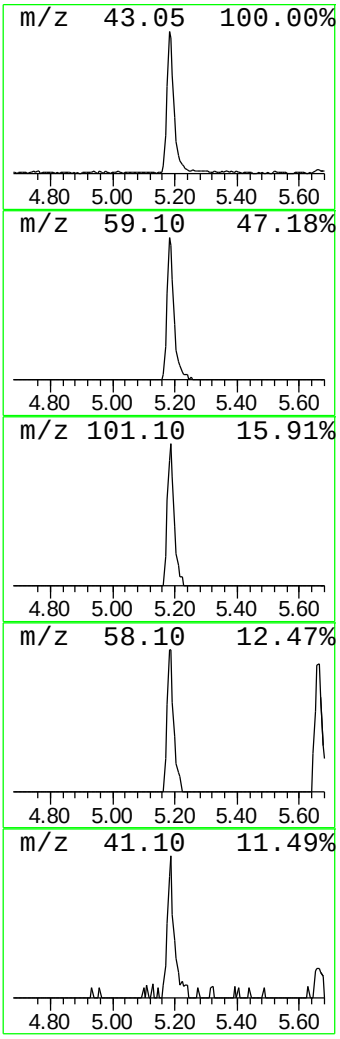
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	7.39 ng	128937	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propylamine	59	C3H9N	000107-10-8	38
4	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	17
5	Butane	58	C4H10	000106-97-8	14





Library Search Compound Report

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Instrument : BNA_M
ClientSampleId : C-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

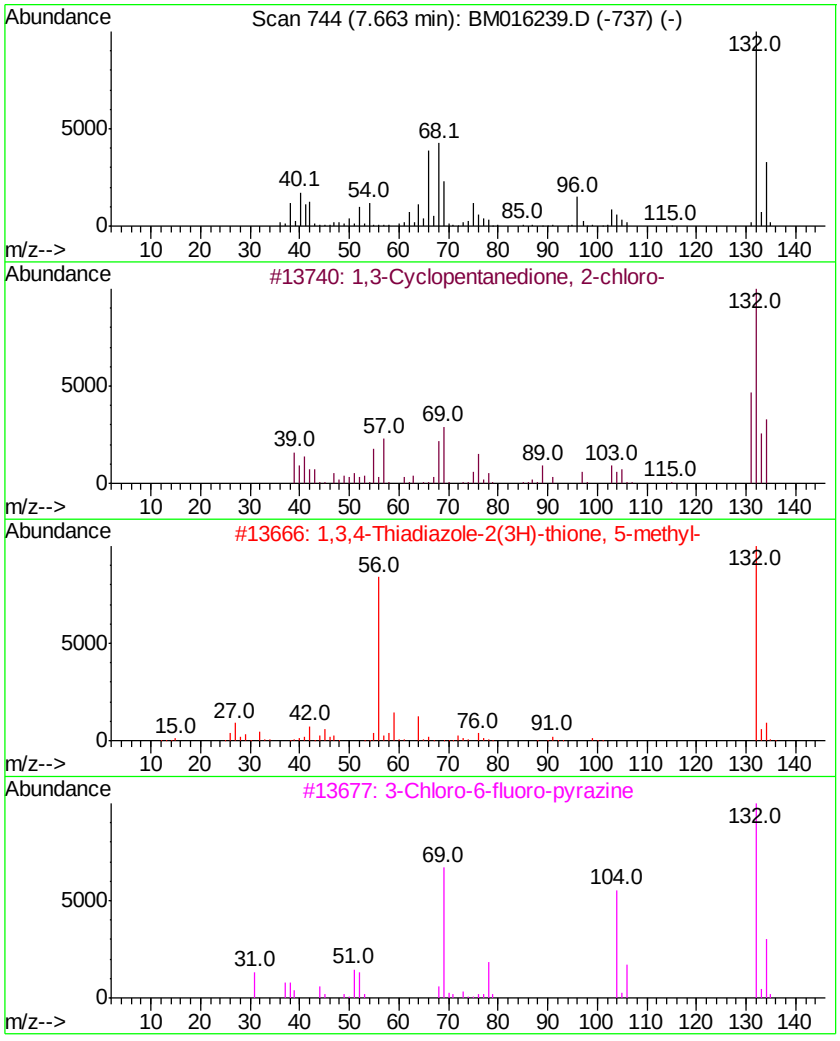
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

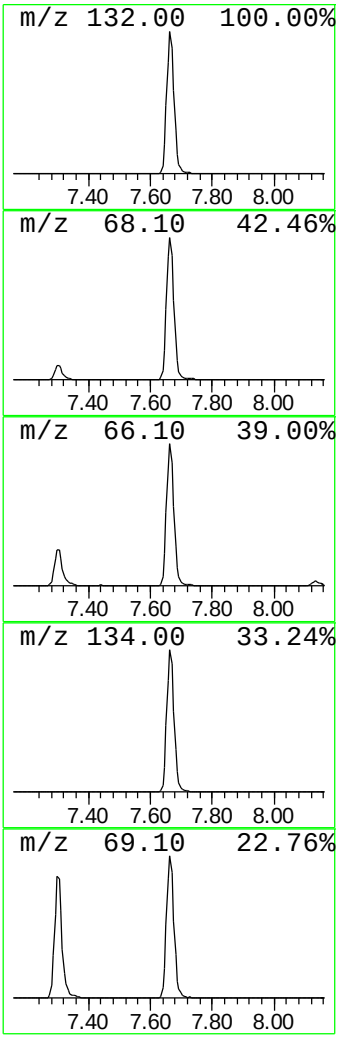
****

Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	66.39 ng	1157800	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14





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Operator : SJ/JU
Sample : J4310-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

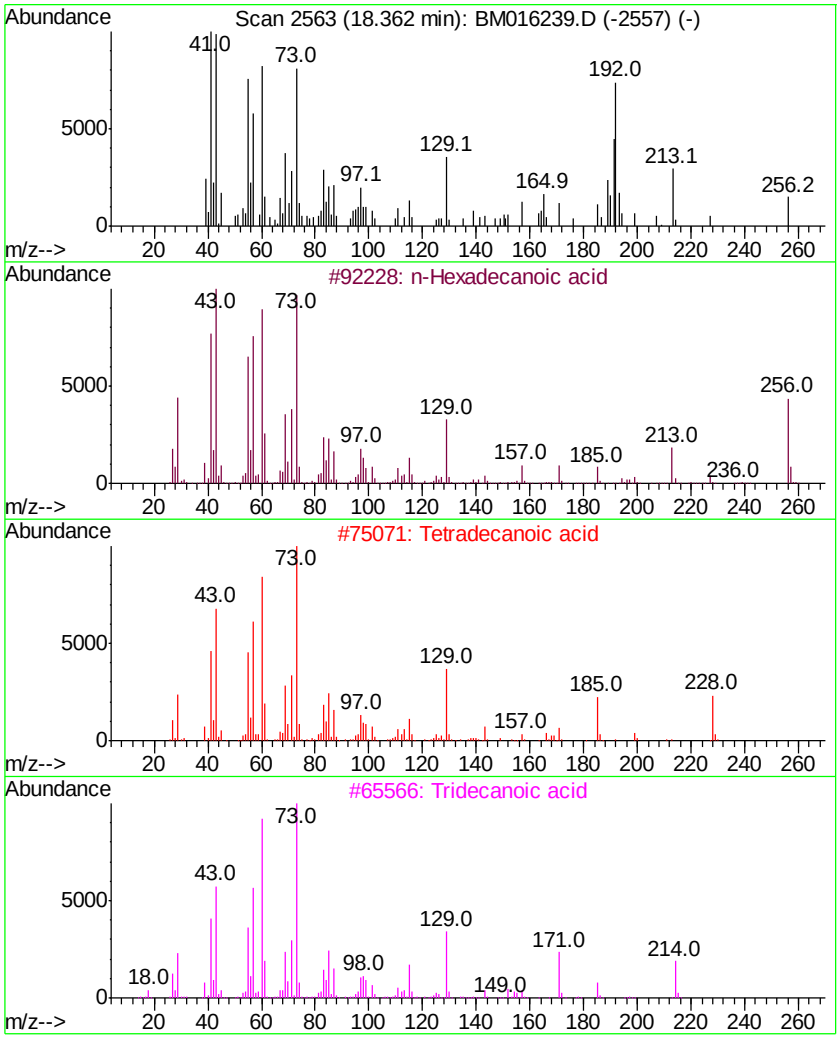
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

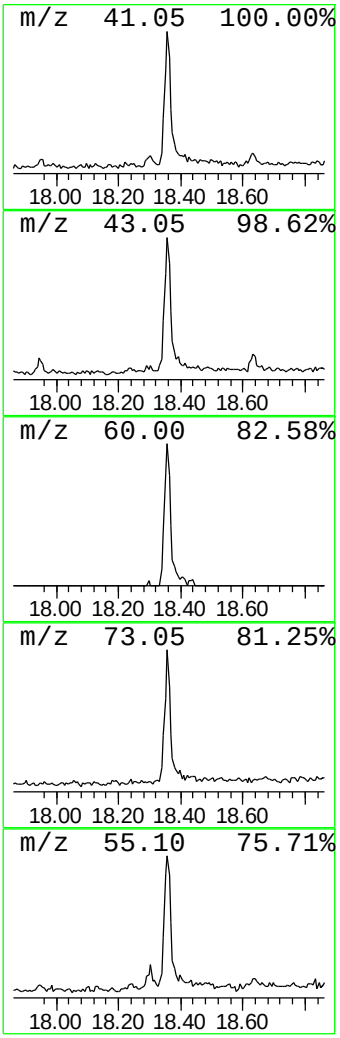
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	6.83 ng	236606	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Tridecanoic acid	214	C13H26O2	000638-53-9	52
4	Undecanoic acid	186	C11H22O2	000112-37-8	50
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50





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Sample : J4310-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

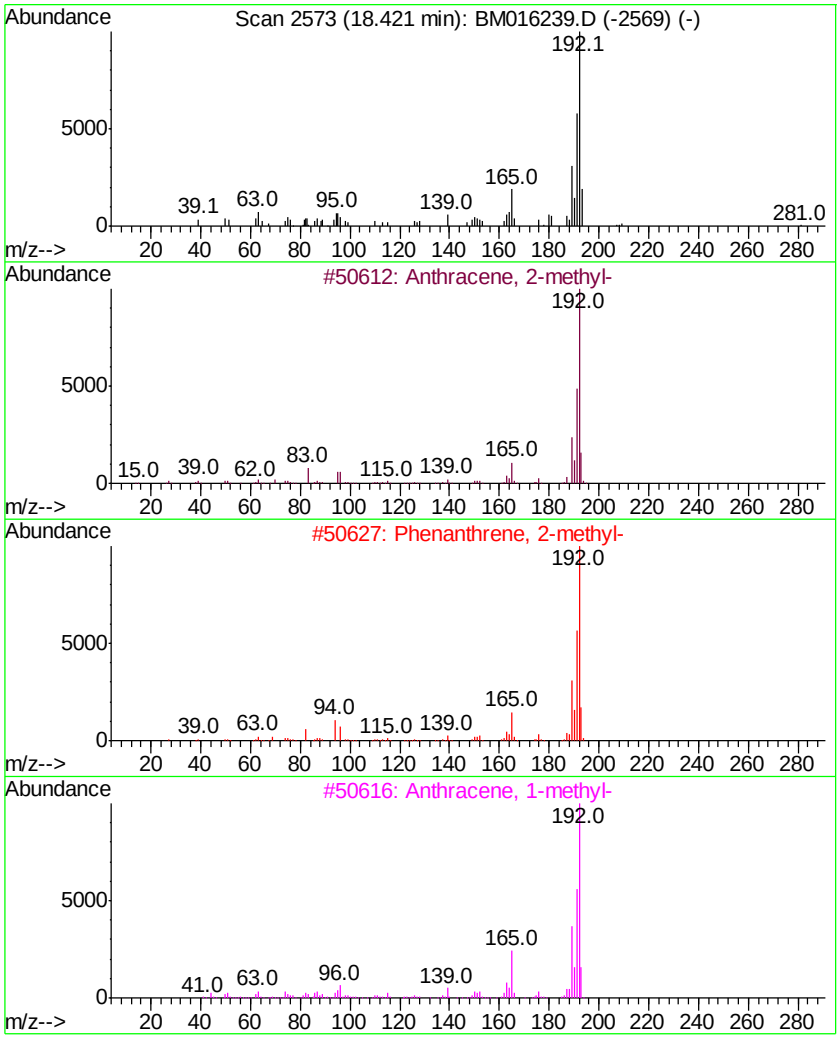
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

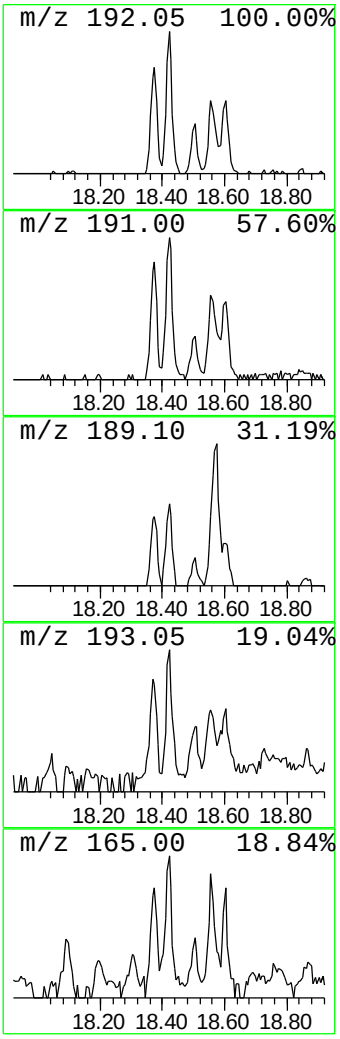
****

Peak Number 5 Anthracene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	3.08 ng	106758	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93





Library Search Compound Report

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Misc :
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Instrument : BNA_M
ClientSampleId : C-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

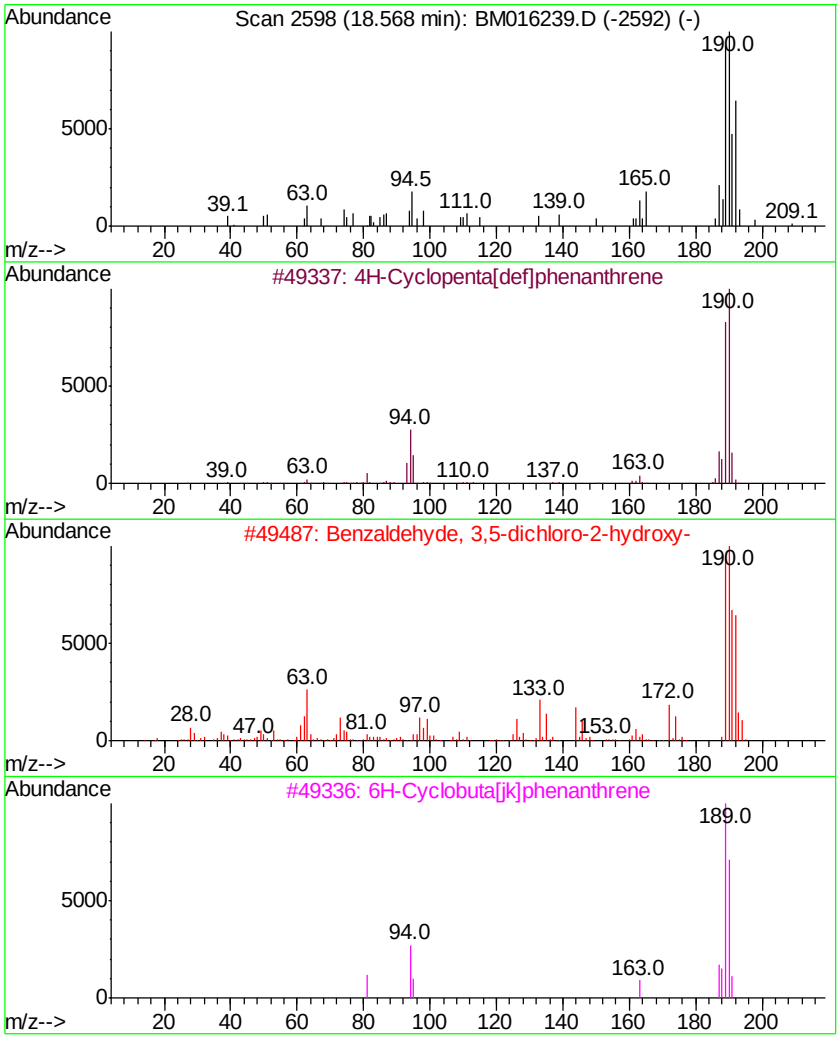
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

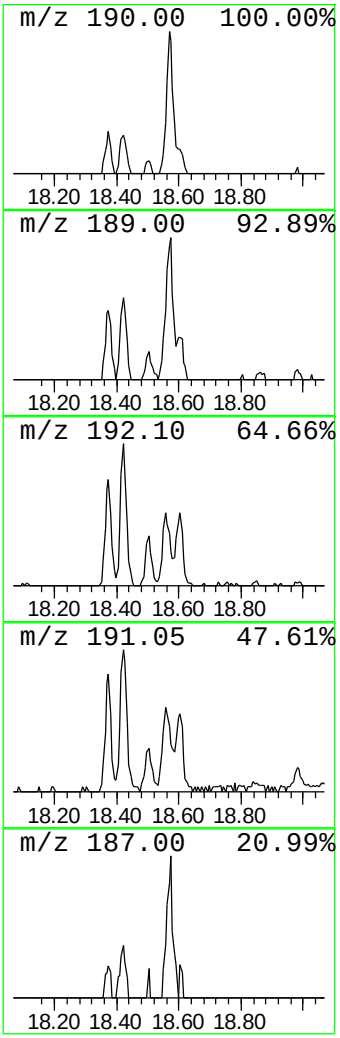
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	2.45 ng	85039	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	40
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	37
4	5-Bromofuroic acid	190	C5H3BrO3	000585-70-6	27
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	18





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Sample : J4310-05
Misc :
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Instrument : BNA_M
ClientSampleId : C-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

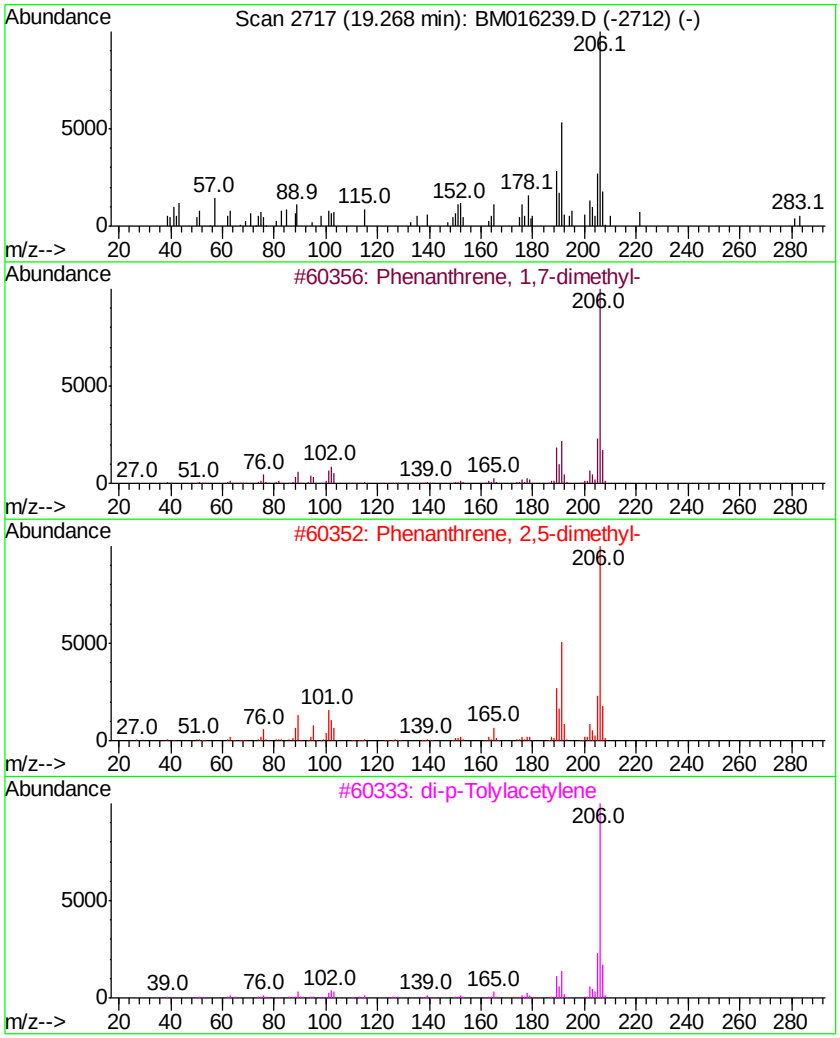
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

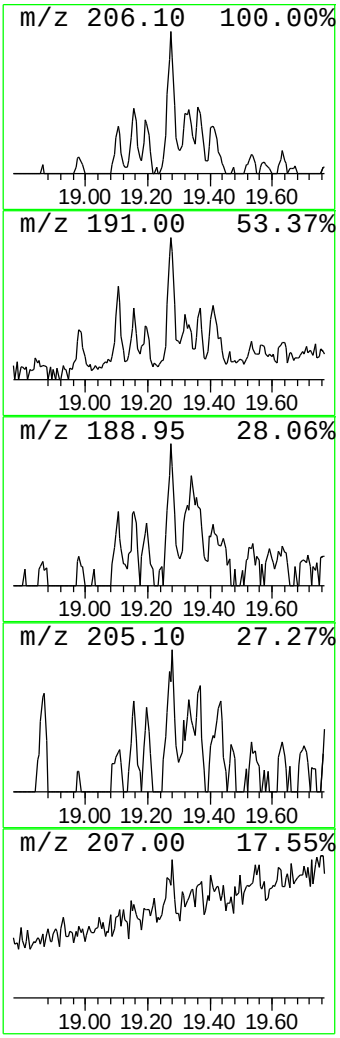
****

Peak Number 7 Phenanthrene, 1,7-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.27	2.20 ng	76396	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	91
2	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	90
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	80
4	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	76
5	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	76





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

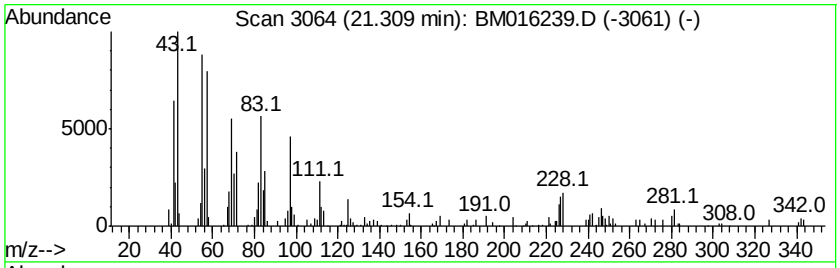
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

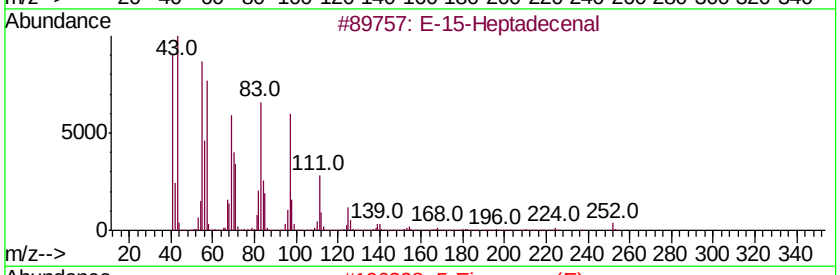
****

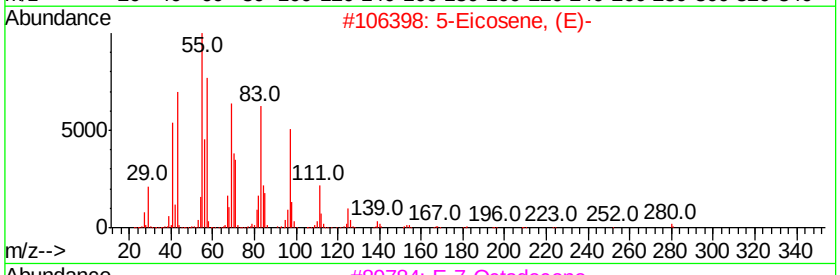
Peak Number 8 E-15-Heptadecenal Concentration Rank 6

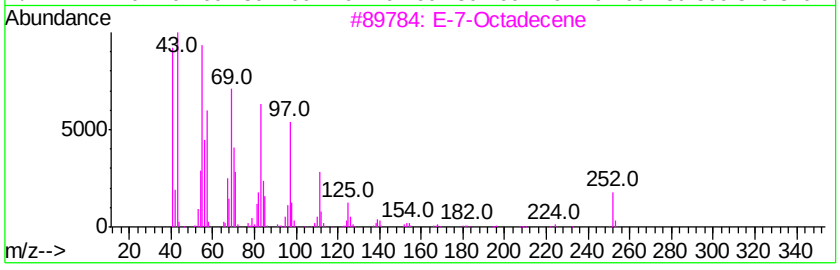
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	3.33 ng	190801	Chrysene-d12	21.64

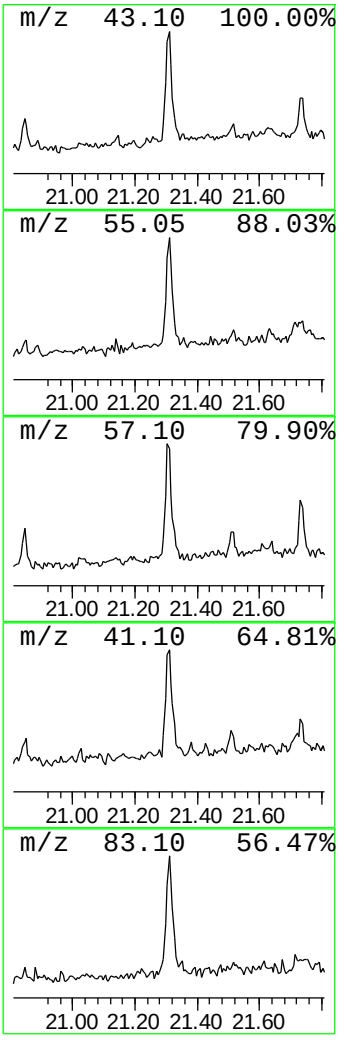
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
3	E-7-Octadecene	252	C18H36	1000130-92-0	93
4	1-Eicosene	280	C20H40	003452-07-1	93
5	1-Octadecene	252	C18H36	000112-88-9	90











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080718\
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Misc :
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Instrument : BNA_M
ClientSampleId : C-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	7.4	ng	128937	1	8.13	348782	20.0
unknown7.66	7.66	66.4	ng	1157800	1	8.13	348782	20.0
n-Hexadecanoic acid	18.36	6.8	ng	236606	4	17.51	693236	20.0
Anthracene, 2-met...	18.42	3.1	ng	106758	4	17.51	693236	20.0
4H-Cyclopenta[def...	18.57	2.5	ng	85039	4	17.51	693236	20.0
Phenanthrene, 1,7...	19.27	2.2	ng	76396	4	17.51	693236	20.0
E-15-Heptadecenal	21.31	3.3	ng	190801	5	21.64	1146850	20.0