LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
Data File : BM017903.D
Acq On : 04 Dec 2018 15:32
Operator : JU/SJ
Sample : J6074-01 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
001-WC-NY5

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-BM111218.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	3.452	76	79	88	rBV	25085	43977	1.42%	0.114%
2	4.769	296	303	308	rBV	60759	83279	2.70%	0.216%
3	5.210	371	378	390	rBV	1538167	2328512	75.39%	6.036%
4	6.769	635	643	664	rBV	1491593	2609572	84.49%	6.765%
5	7.116	695	702	718	rBV	1755284	2733917	88.52%	7.087%
6	7.581	771	781	790	rBV	1016081	1649155	53.40%	4.275%
7	7.893	827	834	842	rBV	1276544	2044776	66.21%	5.301%
8	8.734	969	977	992	rBV	844377	1529423	49.52%	3.965%
9	10.345	1244	1251	1269	rBV	1229413	2222369	71.96%	5.761%
10	12.833	1667	1674	1687	rBV	2016723	3088508	100.00%	8.006%
11	13.698	1815	1821	1835	rBV	183857	340369	11.02%	0.882%
12	14.227	1904	1911	1919	rBV2	1618139	2575963	83.40%	6.678%
13	14.286	1919	1921	1928	rVB4	22921	34585	1.12%	0.090%
14	15.092	2054	2058	2061	rVB2	26174	33626	1.09%	0.087%
15	15.727	2158	2166	2176	rBV	1325168	2112017	68.38%	5.475%
16	15.957	2201	2205	2207	rBV2	36330	55165	1.79%	0.143%
17	16.145	2231	2237	2241	rBV6	19891	31843	1.03%	0.083%
18	16.351	2267	2272	2280	rBV3	35340	66061	2.14%	0.171%
19	16.627	2316	2319	2327	rVB	59803	94955	3.07%	0.246%
20	16.751	2336	2340	2345	rBV4	34405	50071	1.62%	0.130%
21	16.798	2345	2348	2354	rVB4	35375	48844	1.58%	0.127%
22	16.980	2373	2379	2384	rBV	1762941	2591485	83.91%	6.718%
23	17.021	2384	2386	2392	rVB	154454	213186	6.90%	0.553%
24	17.121	2400	2403	2407	rVB	30018	46488	1.51%	0.121%
25	17.310	2429	2435	2440	rBV10	26938	51946	1.68%	0.135%
26	17.486	2462	2465	2471	rBV2	26055	31533	1.02%	0.082%
27	17.892	2526	2534	2543	rBV2	250631	463853	15.02%	1.202%
28	18.051	2557	2561	2565	rBV2	42994	70561	2.28%	0.183%
29	18.180	2580	2583	2586	rBV2	35556	39622	1.28%	0.103%
30	18.374	2612	2616	2620	rBV6	23172	34744	1.12%	0.090%
31	18.780	2683	2685	2689	rVB4	30039	36015	1.17%	0.093%
32	18.821	2689	2692	2700	rBV6	55958	95145	3.08%	0.247%
33	19.051	2726	2731	2734	rBV	261155	370410	11.99%	0.960%
34	19.180	2749	2753	2761	rBV3	150265	245700	7.96%	0.637%

LSC Area Percent Report

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Misc :
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Instrument :
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ClientSampleId :
001-WC-NY5

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-BM111218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.415	2786	2793	2798	rBV	295097	491175	15.90%	1.273%
36	19.627	2824	2829	2835	rBV	2122016	2773336	89.80%	7.189%
37	19.945	2881	2883	2887	rVB	74393	72973	2.36%	0.189%
38	20.445	2966	2968	2971	rVB	101472	89181	2.89%	0.231%
39	20.909	3044	3047	3055	rVB2	357916	485288	15.71%	1.258%
40	21.186	3089	3094	3099	rBV	2099900	2655853	85.99%	6.885%
41	21.345	3119	3121	3125	rVB	224673	209443	6.78%	0.543%
42	21.774	3191	3194	3198	rBV2	261066	338726	10.97%	0.878%
43	22.221	3268	3270	3276	rVB	312528	362044	11.72%	0.939%
44	22.715	3351	3354	3359	rVB3	415175	519179	16.81%	1.346%
45	23.368	3460	3465	3471	rVB2	1383015	2510418	81.28%	6.508%

Sum of corrected areas: 38575291

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
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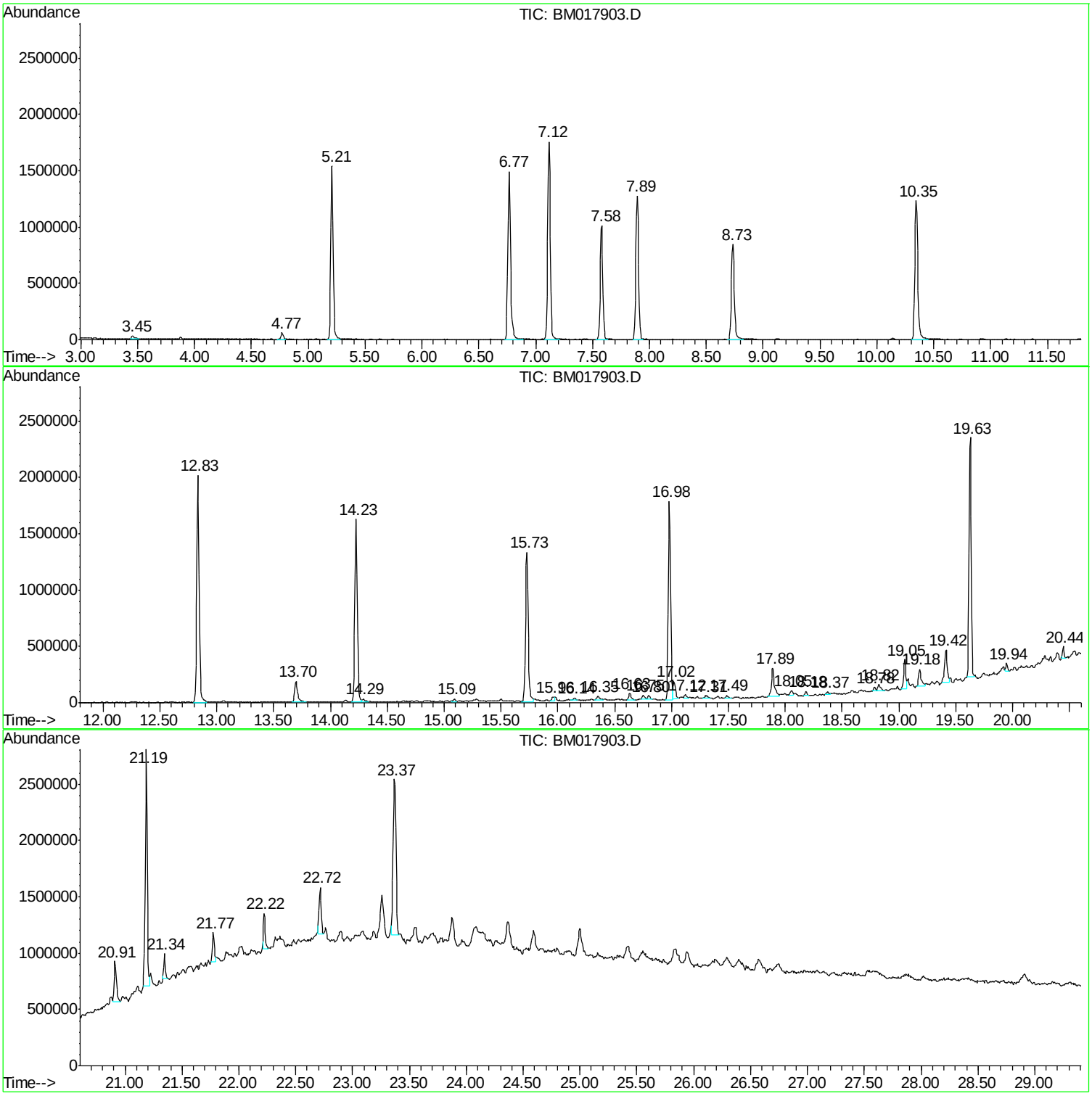
Sample : J6074-01 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
001-WC-NY5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.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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Data File : BM017903.D
Acq On : 04 Dec 2018 15:32
Operator : JU/SJ
Sample : J6074-01 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
001-WC-NY5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

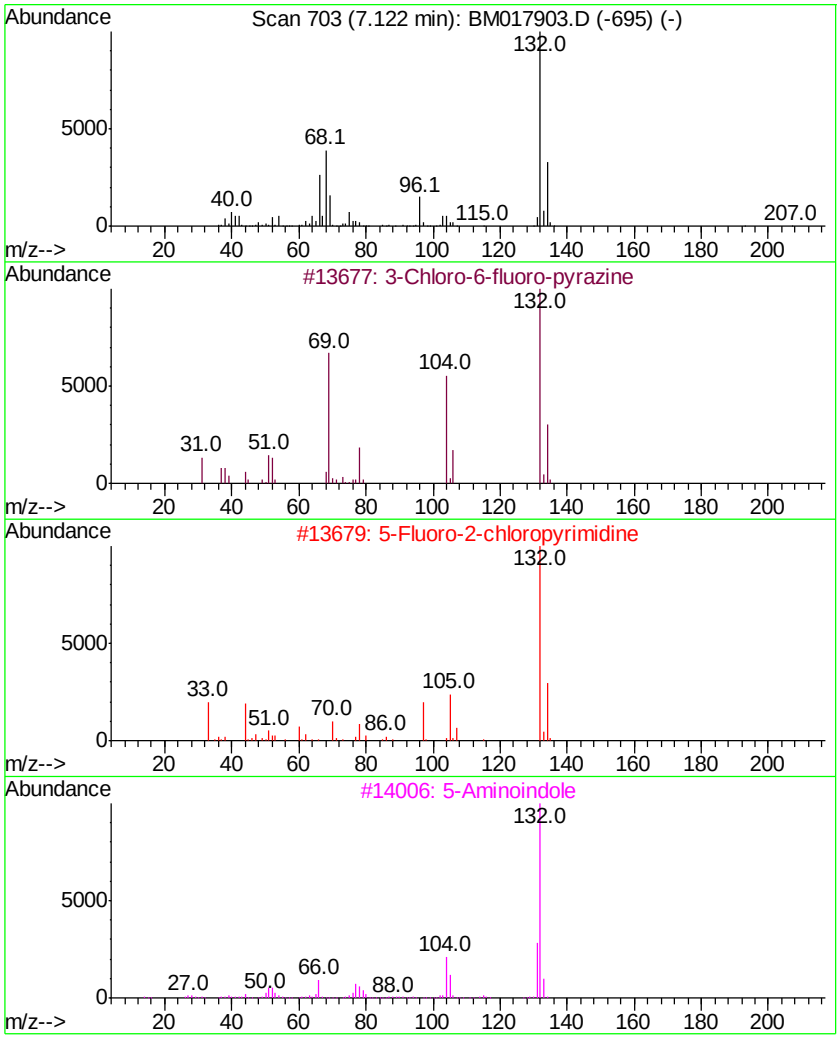
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

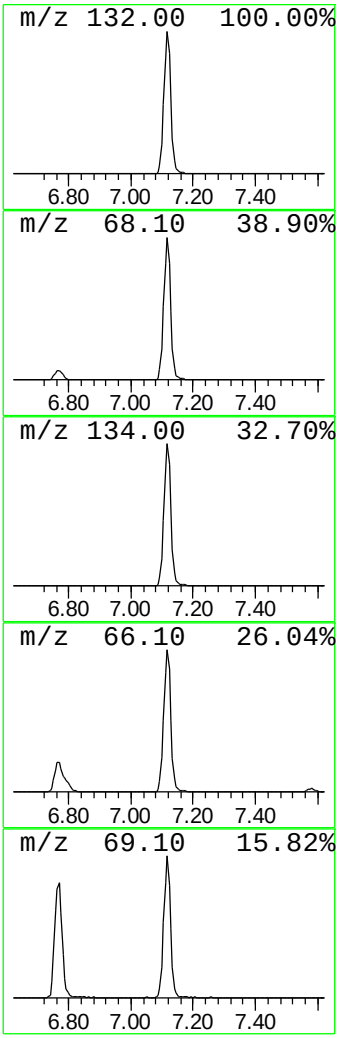
****

Peak Number 1 unknown7.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	33.16 ng	2733920	1,4-Dichlorobenzene-d4	7.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9





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Instrument :
BNA_M
ClientSampleId :
001-WC-NY5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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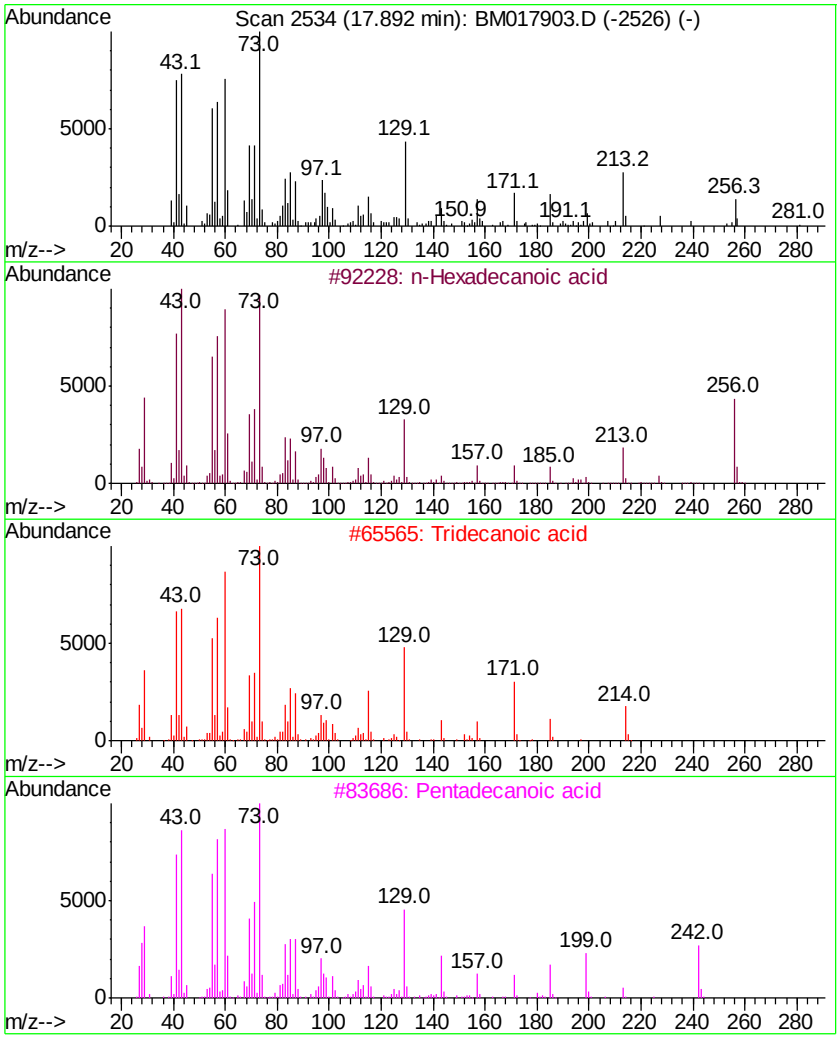
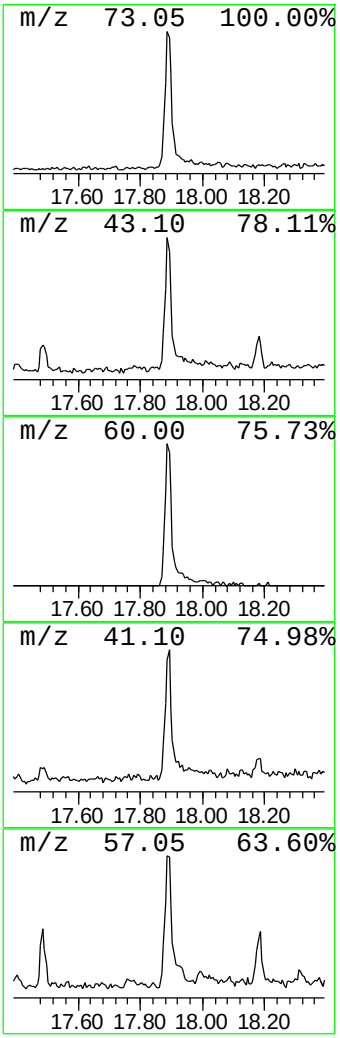
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	3.58 ng	463853	Phenanthrene-d10	16.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68





Library Search Compound Report

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001-WC-NY5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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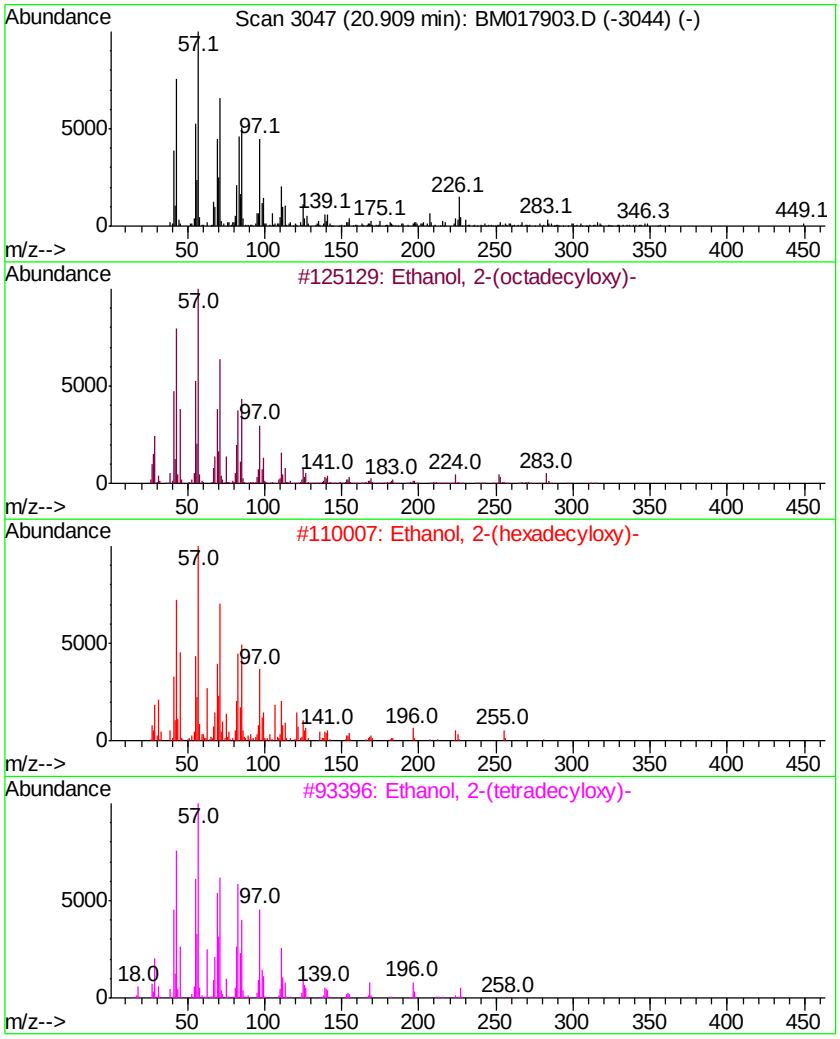
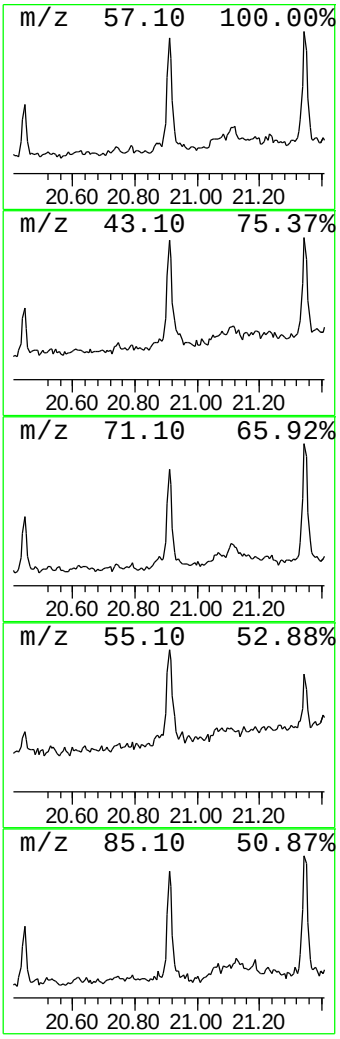
Peak Number 4 Ethanol, 2-(octadecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.91	3.65 ng	485288	Chrysene-d12	21.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	87
2	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	83
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	74
4	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	64
5	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	64





Library Search Compound Report

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Instrument :
BNA_M
ClientSampleId :
001-WC-NY5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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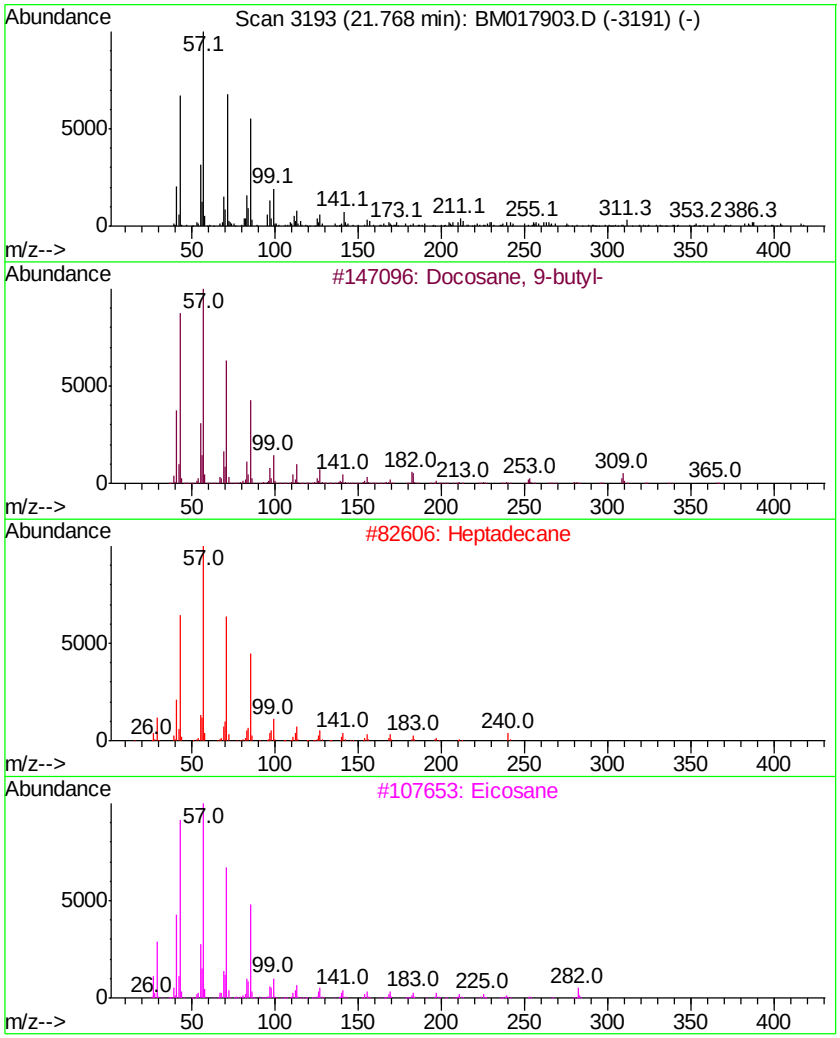
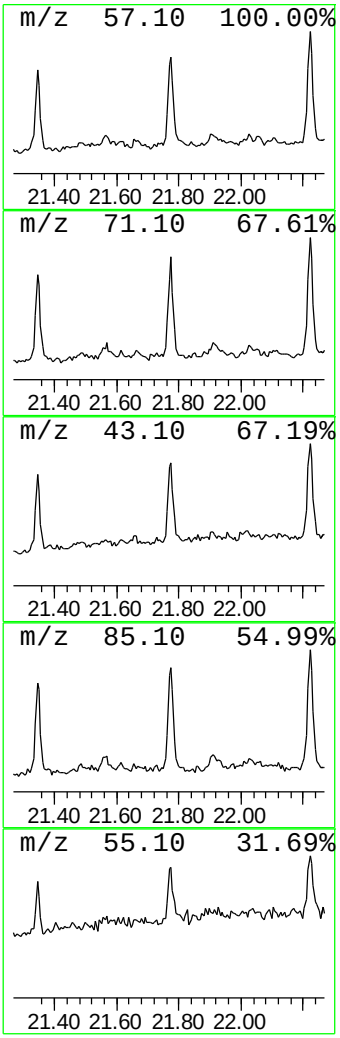
Peak Number 5 Docosane, 9-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.77	2.55 ng	338726	Chrysene-d12	21.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 9-butyl-	366	C26H54	055282-14-9	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Pentacosane	352	C25H52	000629-99-2	90





Library Search Compound Report

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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM111218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

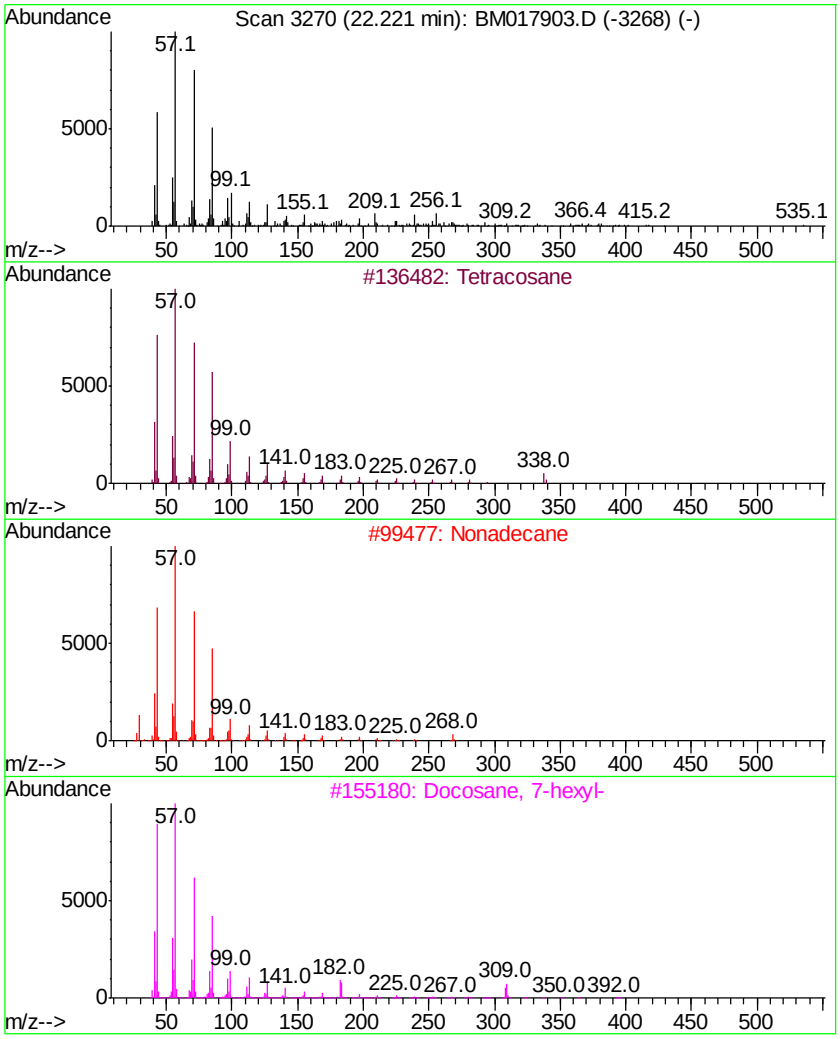
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

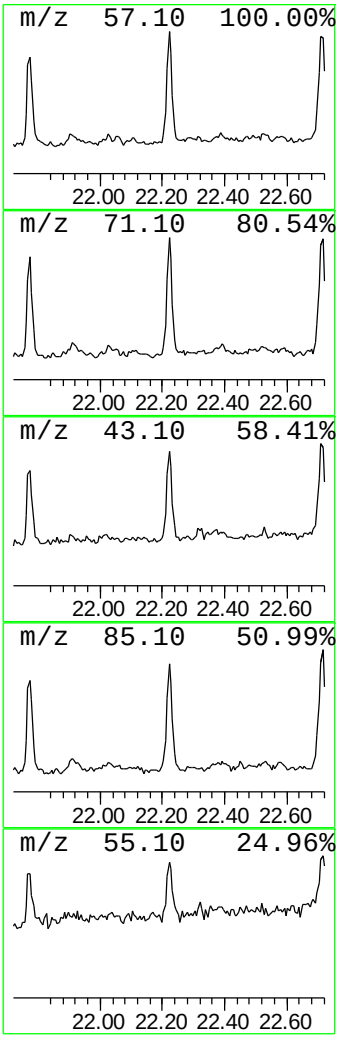
****

Peak Number 6 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.22	2.73 ng	362044	Chrysene-d12	21.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Nonadecane	268	C19H40	000629-92-5	94
3	Docosane, 7-hexyl-	394	C28H58	055373-86-9	94
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	93
5	Pentacosane	352	C25H52	000629-99-2	91





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
unknown7.12	7.12	33.2	ng	2733920	1	7.58	1649160	20.0
n-Hexadecanoic acid	17.89	3.6	ng	463853	4	16.98	2591490	20.0
Ethanol, 2-(octad...	20.91	3.6	ng	485288	5	21.19	2655850	20.0
Docosane, 9-butyl-	21.77	2.5	ng	338726	5	21.19	2655850	20.0
Tetracosane	22.22	2.7	ng	362044	5	21.19	2655850	20.0