LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM103017\
Data File : BM012589.D
Acq On : 31 Oct 2017 00:37
Operator : SJ/JU
Sample : I5886-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : ESNE7

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.140	6	9	16	rVB2	58403	81459	1.19%	0.102%
2	3.351	41	45	52	rVB	59280	82699	1.21%	0.104%
3	3.863	127	132	136	rBV	57681	82328	1.21%	0.103%
4	4.987	317	323	333	rVB2	47538	96912	1.42%	0.122%
5	7.022	662	669	682	rVB2	889077	1636529	23.96%	2.052%
6	7.187	689	697	706	rBV	702764	1072476	15.70%	1.345%
7	7.392	725	732	741	rVB	914035	1475547	21.60%	1.850%
8	7.857	803	811	819	rBV	1301010	2078732	30.43%	2.607%
9	8.557	920	930	939	rBV	1018070	1676683	24.54%	2.103%
10	9.010	999	1007	1015	rBV	829744	1375229	20.13%	1.725%
11	9.728	1122	1129	1136	rBV	681868	1137425	16.65%	1.426%
12	10.269	1214	1221	1230	rBV	1103124	1861146	27.24%	2.334%
13	10.645	1274	1285	1292	rBV	1657501	2780355	40.70%	3.487%
14	10.780	1301	1308	1319	rBV	438577	821977	12.03%	1.031%
15	11.963	1502	1509	1520	rBV	91616	162220	2.37%	0.203%
16	13.892	1827	1837	1842	rBV	1838123	2542124	37.21%	3.188%
17	13.939	1842	1845	1849	rVB	121290	156145	2.29%	0.196%
18	14.180	1874	1886	1897	rBV	2113326	3160255	46.26%	3.963%
19	14.315	1903	1909	1918	rBV2	49172	93329	1.37%	0.117%
20	14.486	1929	1938	1946	rBV2	2420252	3705056	54.24%	4.646%
21	14.686	1964	1972	1981	rBV	675078	1108877	16.23%	1.391%
22	14.768	1983	1986	1993	rVB	38504	69136	1.01%	0.087%
23	14.898	2001	2008	2014	rVB8	42329	77870	1.14%	0.098%
24	15.186	2053	2057	2067	rVB2	80089	143823	2.11%	0.180%
25	15.474	2100	2106	2113	rBV	2692711	3828669	56.05%	4.801%
26	15.539	2113	2117	2122	rVV6	55003	84487	1.24%	0.106%
27	15.598	2122	2127	2136	rVV	709704	948918	13.89%	1.190%
28	15.839	2162	2168	2173	rBV	443878	627452	9.19%	0.787%
29	16.198	2223	2229	2230	rBV3	68096	75332	1.10%	0.094%
30	16.221	2231	2233	2238	rVB	110224	137549	2.01%	0.172%
31	16.627	2296	2302	2306	rBV5	45598	86702	1.27%	0.109%
32	16.768	2320	2326	2331	rBV10	35081	71564	1.05%	0.090%
33	16.998	2360	2365	2370	rBV3	103236	225959	3.31%	0.283%
34	17.045	2370	2373	2380	rVB4	60279	99391	1.45%	0.125%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM103017\
Data File : BM012589.D
Acq On : 31 Oct 2017 00:37
Operator : SJ/JU
Sample : I5886-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : ESNE7

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Title : SVOA CALIBRATION

35	17.227	2398	2404	2408	rBV2	3308218	4547093	66.56%	5.702%
36	17.268	2408	2411	2415	rVV	493057	657813	9.63%	0.825%
37	17.327	2415	2421	2431	rVB2	2706189	4028765	58.98%	5.052%
38	17.727	2485	2489	2497	rBV3	48942	81858	1.20%	0.103%
39	18.121	2549	2556	2559	rBV2	533638	811579	11.88%	1.018%
40	18.292	2581	2585	2589	rBV3	79448	133742	1.96%	0.168%
41	18.327	2589	2591	2596	rVB2	54310	76021	1.11%	0.095%
42	18.603	2634	2638	2641	rBV	76523	99468	1.46%	0.125%
43	18.639	2641	2644	2648	rBV2	105269	135683	1.99%	0.170%
44	19.156	2729	2732	2738	rVB	74367	111500	1.63%	0.140%
45	19.280	2745	2753	2759	rBV	1245068	1724447	25.24%	2.163%
46	19.397	2769	2773	2778	rBV2	290657	414048	6.06%	0.519%
47	19.615	2804	2810	2813	rBV	3714340	5136156	75.19%	6.441%
48	21.109	3061	3064	3071	rVB3	794496	1008853	14.77%	1.265%
49	21.315	3096	3099	3104	rBV	239169	258945	3.79%	0.325%
50	21.397	3107	3113	3117	rVV	4810095	6831157	100.00%	8.567%
51	21.433	3117	3119	3131	rVB	718790	1078635	15.79%	1.353%
52	22.156	3237	3242	3251	rBV	2713647	3740171	54.75%	4.690%
53	22.997	3380	3385	3388	rBV3	1007704	1886433	27.62%	2.366%
54	23.038	3388	3392	3399	rVB2	1644869	2907990	42.57%	3.647%
55	23.550	3473	3479	3485	rBV2	2505544	4902837	71.77%	6.148%
56	23.697	3498	3504	3511	rBV	2944714	5503407	80.56%	6.902%

Sum of corrected areas: 79740956

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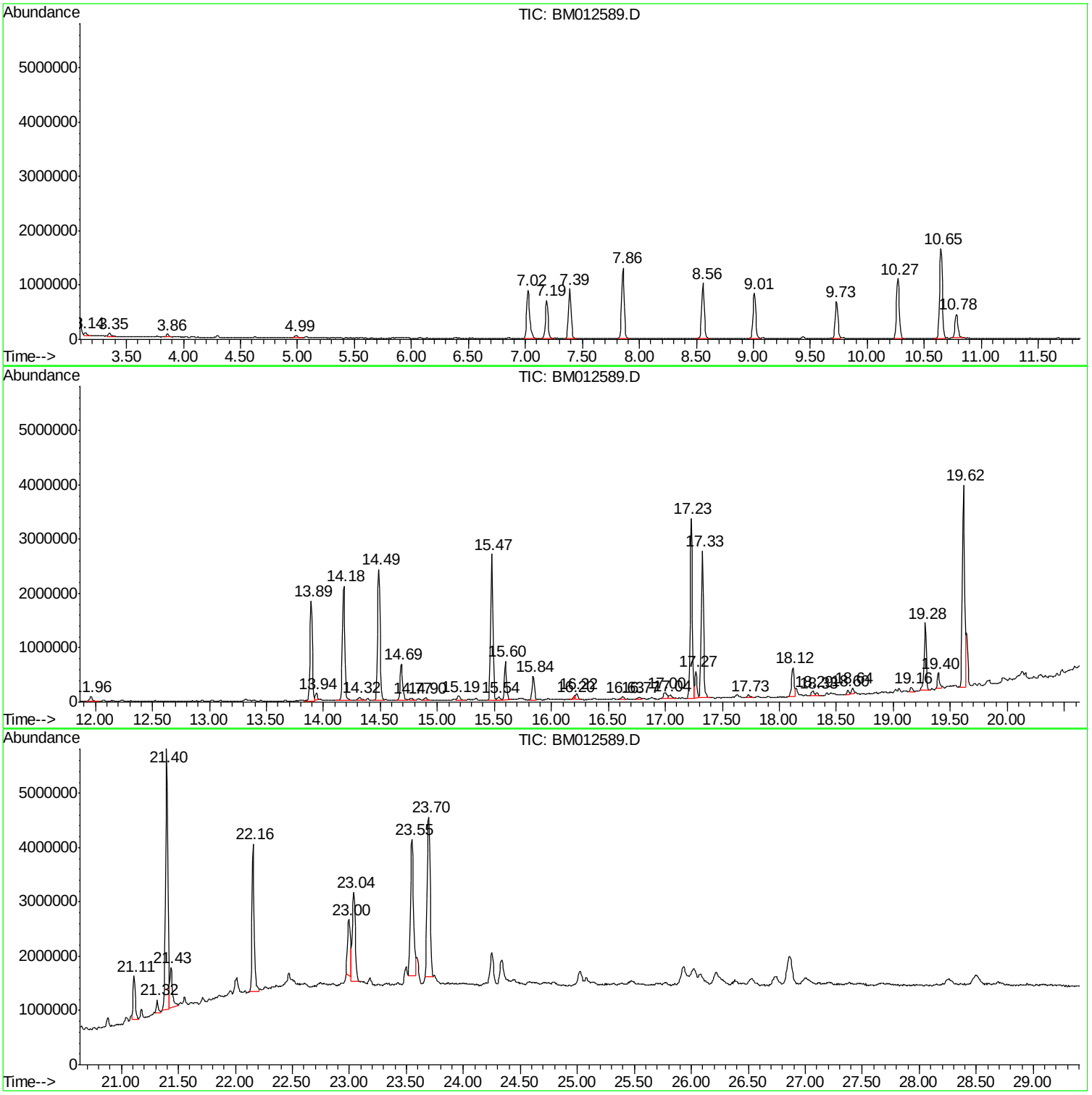
Instrument :
BNA_M
ClientSampleId :
ESNE7

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

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



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Acq On : 31 Oct 2017 00:37
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Sample : I5886-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : ESNE7

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

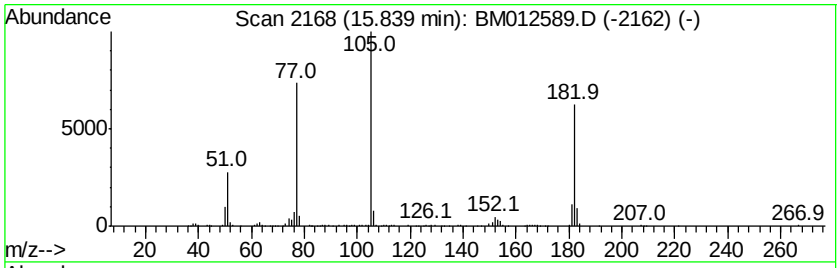
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

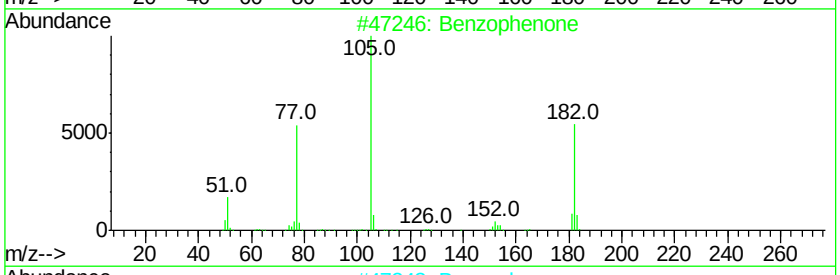
****

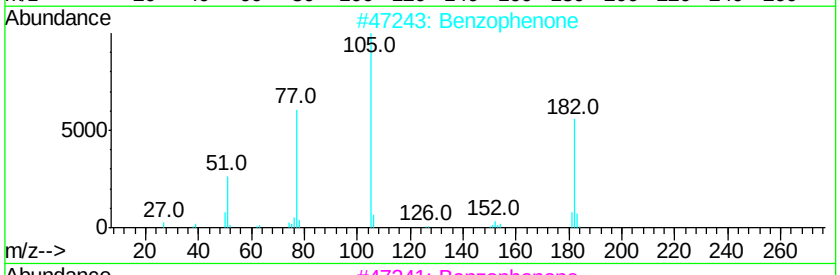
Peak Number 1 Benzophenone Concentration Rank 3

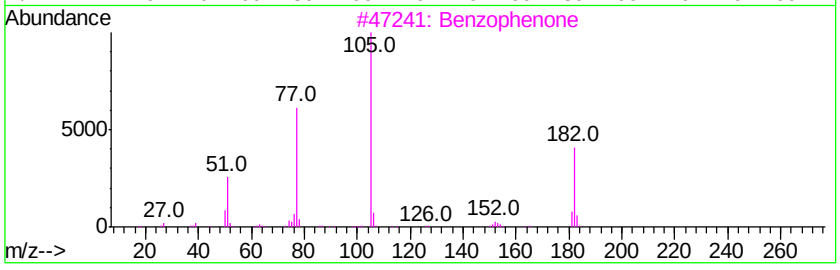
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	3.39 ng/ul	627452	Acenaphthene-d10	14.49

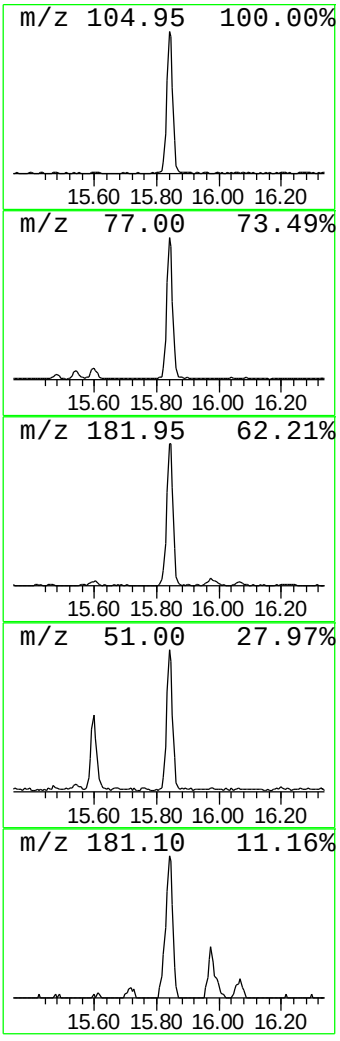
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzophenone	182	C13H10O	000119-61-9	96
3	Benzophenone	182	C13H10O	000119-61-9	94
4	Benzophenone	182	C13H10O	000119-61-9	94
5	Benzophenone	182	C13H10O	000119-61-9	91











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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : ESNE7

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

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

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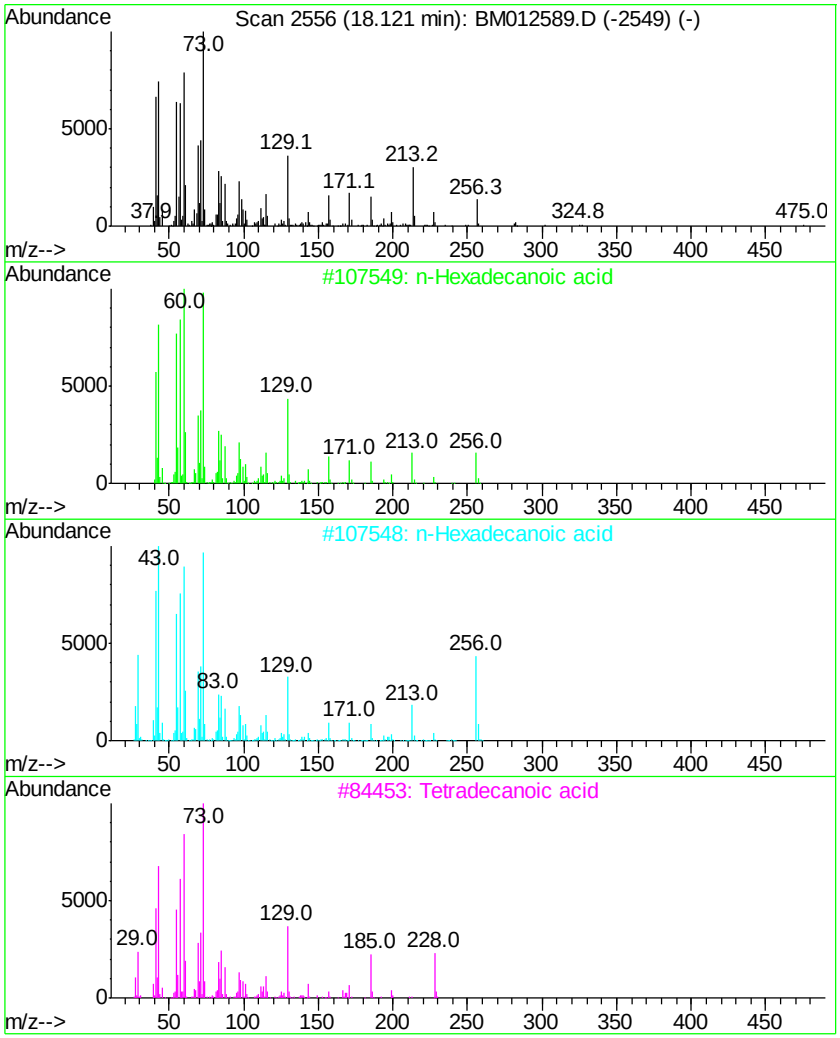
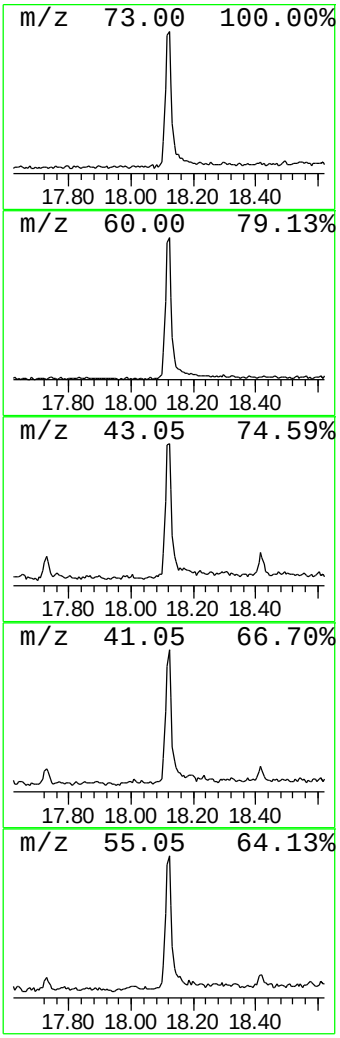
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.12	3.57 ng/ul	811579	Phenanthrene-d10	17.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Octadecanoic acid	284	C18H36O2	000057-11-4	93
5	Tridecanoic acid	214	C13H26O2	000638-53-9	91





Data Path : Z:\HPCHEM1\BNA M\DATA\BM103017\
Data File : BM012589.D
Acq On : 31 Oct 2017 00:37
Operator : SJ/JU
Sample : I5886-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : ESNE7

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

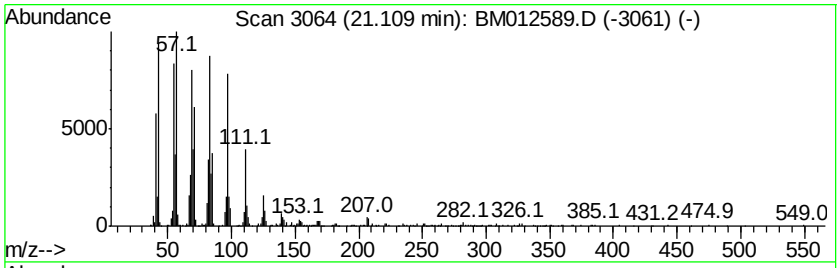
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

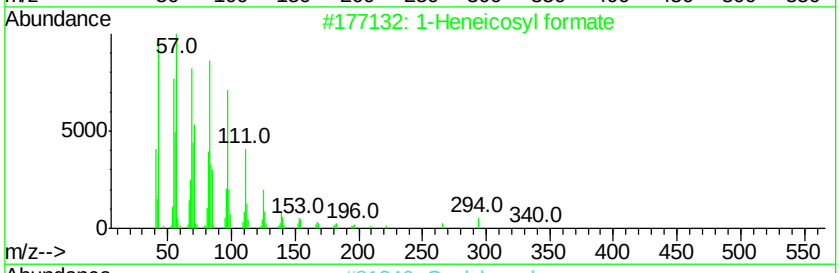
****

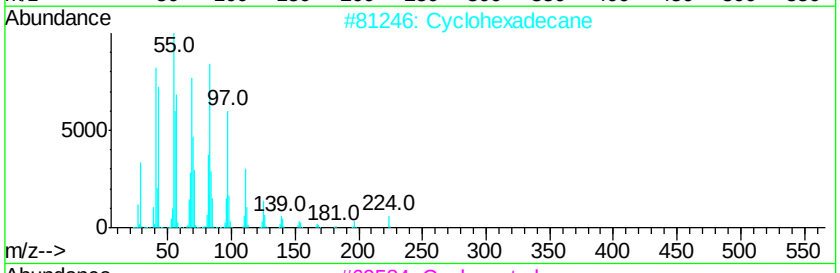
Peak Number 3 1-Heneicosyl formate Concentration Rank 4

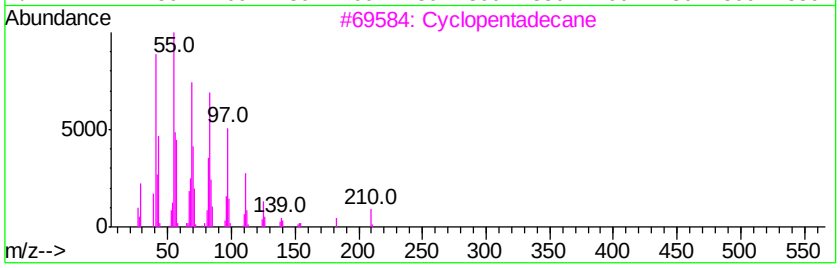
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.11	2.95 ng/ul	1008850	Chrysene-d12	21.40

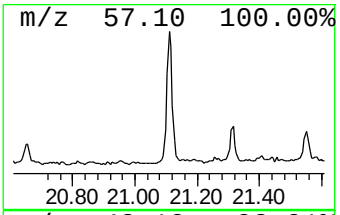
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	99
2	Cyclohexadecane	224	C16H32	000295-65-8	93
3	Cyclopentadecane	210	C15H30	000295-48-7	93
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90

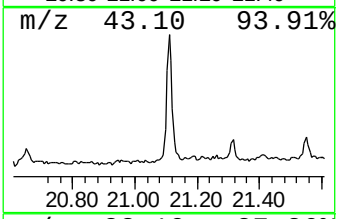


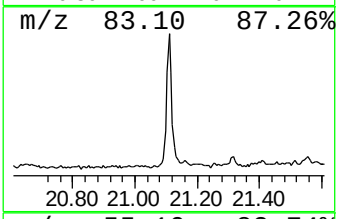


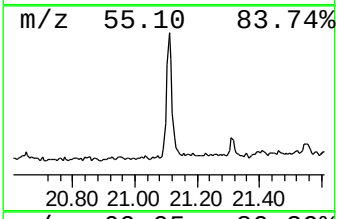


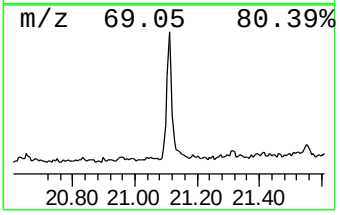












Library Search Compound Report

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Instrument : BNA_M
ClientSampleId : ESNE7

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

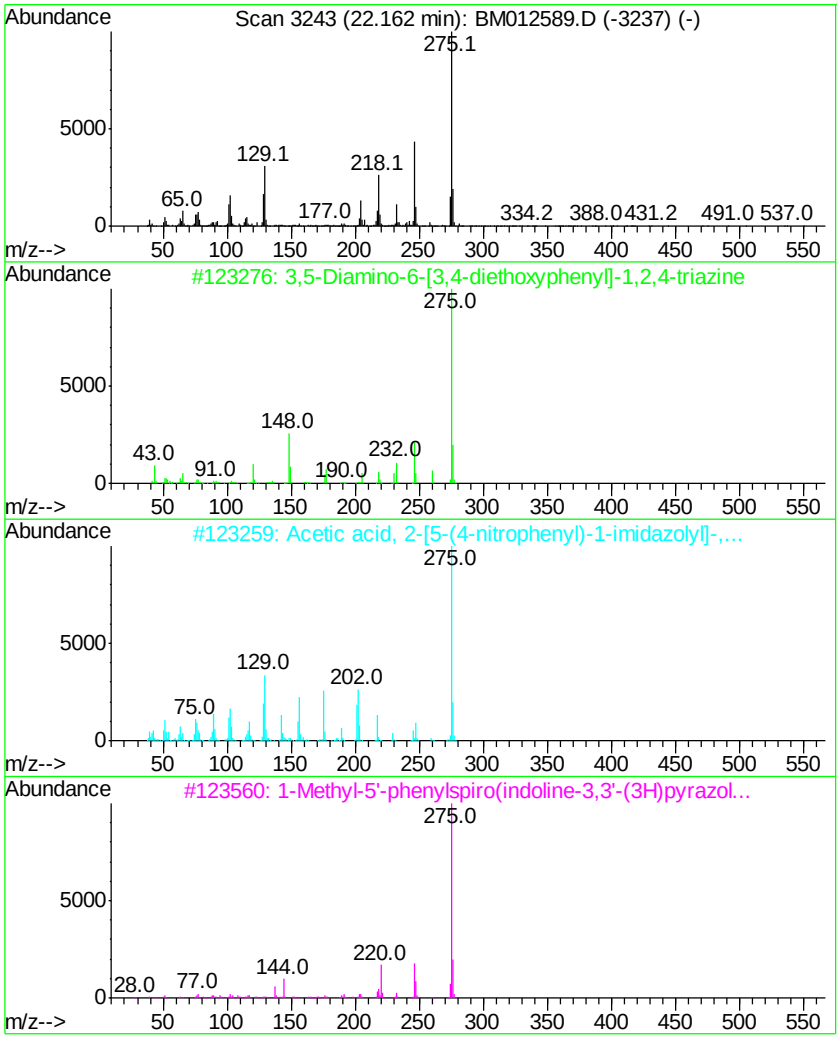
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

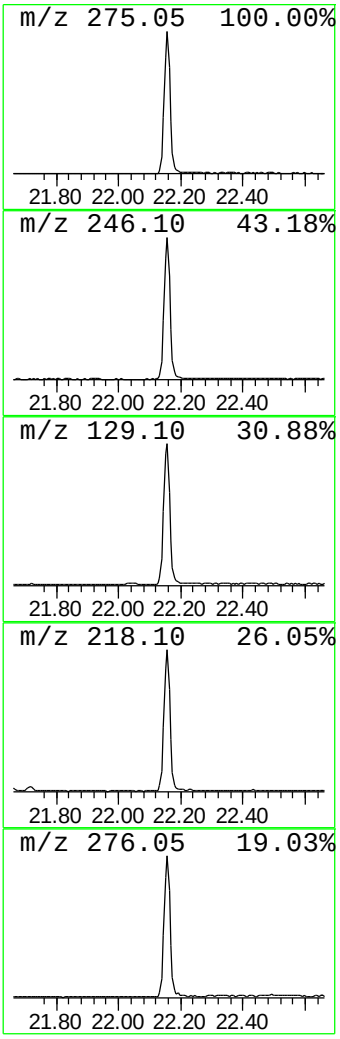
****

Peak Number 4 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.16	10.95 ng/ul	3740170	Chrysene-d12	21.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Diamino-6-[3,4-diethoxyphenv...	275	C13H17N5O2	058848-69-4	47
2	Acetic acid, 2-[5-(4-nitrophenyl...	275	C13H13N3O4	351064-45-4	47
3	1-Methyl-5'-phenylspiro(indoline...	275	C17H13N3O	015970-21-5	43
4	5H-[1]Benzopyrano[4,3-d]pyrimidi...	275	C16H9N3O2	1000337-49-1	41
5	8H-Benzo[g]-1,3-benzodioxolo[6,5...	275	C17H9NO3	000475-75-2	38





Tentatively Identified Compound (LSC) summary

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Quant Title : SVOA 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
Benzophenone	15.84	3.4	ng/ul	627452	3	14.49	3705060	20.0
n-Hexadecanoic acid	18.12	3.6	ng/ul	811579	4	17.23	4547090	20.0
1-Heneicosyl formate	21.11	3.0	ng/ul	1008850	5	21.40	6831160	20.0
unknown-01	22.16	10.9	ng/ul	3740170	5	21.40	6831160	20.0