LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
Data File : BM017912.D
Acq On : 04 Dec 2018 20:59
Operator : JU/SJ
Sample : J5770-15 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : OR-03-112918-B

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	4.769	296	303	312	rBV	85252	134569	3.12%	0.270%
2	5.210	371	378	395	rBV	1989925	2939055	68.16%	5.888%
3	6.775	636	644	658	rBV	1928179	3396123	78.76%	6.804%
4	7.122	695	703	714	rBV	2198077	3465306	80.36%	6.942%
5	7.581	772	781	791	rBV	1105619	1718262	39.85%	3.442%
6	7.893	827	834	847	rVB	1624400	2668871	61.89%	5.347%
7	8.734	969	977	990	rBV	1152706	1989234	46.13%	3.985%
8	10.351	1243	1252	1268	rBV	1284964	2323446	53.88%	4.655%
9	12.245	1567	1574	1584	rVB2	33165	66202	1.54%	0.133%
10	12.839	1668	1675	1687	rBV	2904826	4312011	100.00%	8.639%
11	13.545	1789	1795	1799	rBV2	43888	71575	1.66%	0.143%
12	13.698	1815	1821	1827	rBV	164994	283505	6.57%	0.568%
13	13.951	1856	1864	1872	rBV	104561	184444	4.28%	0.370%
14	14.227	1904	1911	1918	rBV2	1728783	2626106	60.90%	5.261%
15	14.292	1918	1922	1931	rVB	54544	97326	2.26%	0.195%
16	14.633	1976	1980	1985	rBV2	36984	57200	1.33%	0.115%
17	14.851	2011	2017	2023	rBV4	24171	56271	1.30%	0.113%
18	15.286	2084	2091	2103	rVB2	65901	141720	3.29%	0.284%
19	15.727	2158	2166	2175	rBV	1761977	2730120	63.31%	5.469%
20	15.974	2201	2208	2214	rVB7	38387	81409	1.89%	0.163%
21	16.292	2256	2262	2267	rBV9	30100	67551	1.57%	0.135%
22	16.804	2346	2349	2357	rVB3	50999	90330	2.09%	0.181%
23	16.986	2374	2380	2384	rBV	1812825	2561906	59.41%	5.132%
24	17.027	2384	2387	2394	rVV	436486	616396	14.29%	1.235%
25	17.121	2398	2403	2409	rVV	132934	205832	4.77%	0.412%
26	17.192	2409	2415	2418	rVB6	23361	44421	1.03%	0.089%
27	17.404	2447	2451	2456	rBV3	30152	54146	1.26%	0.108%
28	17.862	2524	2529	2531	rBV	91738	138907	3.22%	0.278%
29	17.892	2531	2534	2542	rVV3	368674	661442	15.34%	1.325%
30	17.962	2543	2546	2549	rVV	59868	88083	2.04%	0.176%
31	17.992	2549	2551	2556	rVV	51169	72633	1.68%	0.146%
32	18.057	2557	2562	2566	rVV2	129367	254642	5.91%	0.510%
33	18.092	2566	2568	2576	rVB2	66427	100508	2.33%	0.201%
34	18.368	2612	2615	2620	rBV	50932	81699	1.89%	0.164%

LSC Area Percent Report

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Data File : BM017912.D
Acq On : 04 Dec 2018 20:59
Operator : JU/SJ
Sample : J5770-15 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : OR-03-112918-B

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	18.421	2620	2624	2628	rVB3	39671	60959	1.41%	0.122%
36	18.786	2683	2686	2690	rBV	84030	115446	2.68%	0.231%
37	18.933	2707	2711	2718	rBV6	44265	100392	2.33%	0.201%
38	19.051	2726	2731	2738	rBV	787012	1144832	26.55%	2.294%
39	19.186	2750	2754	2757	rBV3	127525	199055	4.62%	0.399%
40	19.415	2785	2793	2803	rBV	746554	1229328	28.51%	2.463%
41	19.498	2804	2807	2814	rVB2	49809	81389	1.89%	0.163%
42	19.627	2824	2829	2840	rVB	3143544	4053616	94.01%	8.121%
43	19.762	2846	2852	2857	rBV2	60581	150658	3.49%	0.302%
44	19.921	2876	2879	2883	rVB	133069	163902	3.80%	0.328%
45	20.021	2893	2896	2900	rBV2	99598	118561	2.75%	0.238%
46	20.915	3044	3048	3054	rBV2	423238	602702	13.98%	1.207%
47	21.192	3089	3095	3099	rBV2	2206189	3358016	77.88%	6.727%
48	21.227	3099	3101	3108	rVB	442301	520122	12.06%	1.042%
49	22.721	3351	3355	3361	rBV2	559589	1174860	27.25%	2.354%
50	23.374	3461	3466	3472	rBV	1380223	2460895	57.07%	4.930%

Sum of corrected areas: 49915984

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
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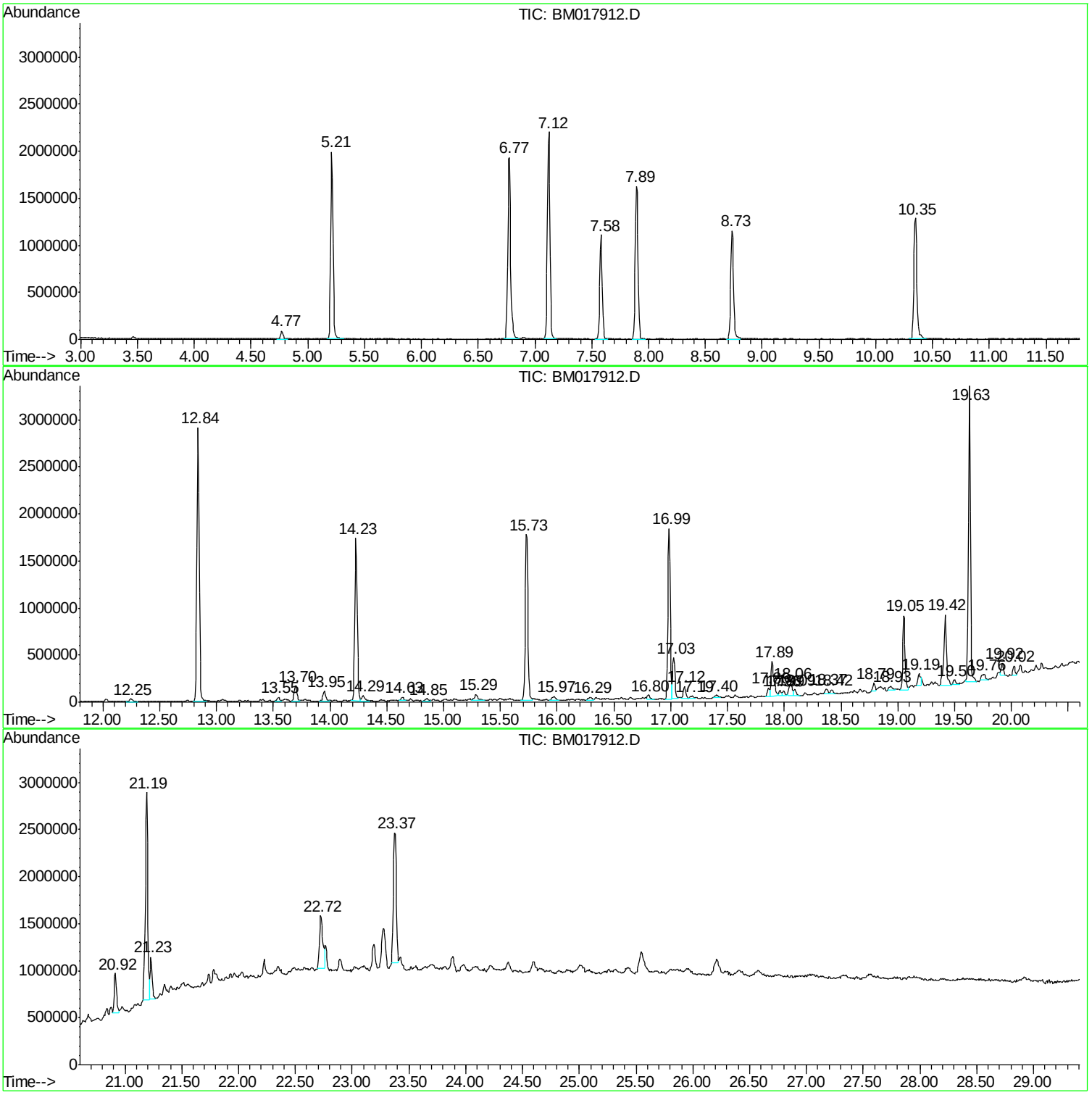
Acq On : 04 Dec 2018 20:59
Operator : JU/SJ
Sample : J5770-15 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : OR-03-112918-B

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
Data File : BM017912.D
Acq On : 04 Dec 2018 20:59
Operator : JU/SJ
Sample : J5770-15 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : OR-03-112918-B

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

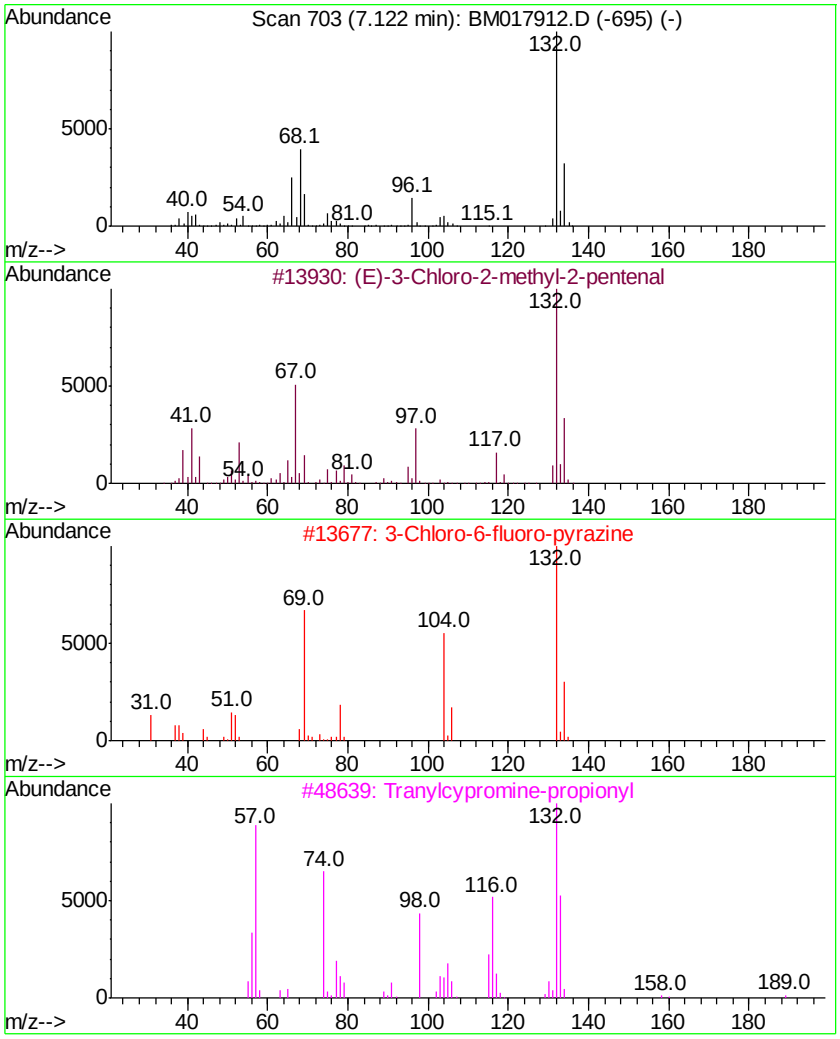
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

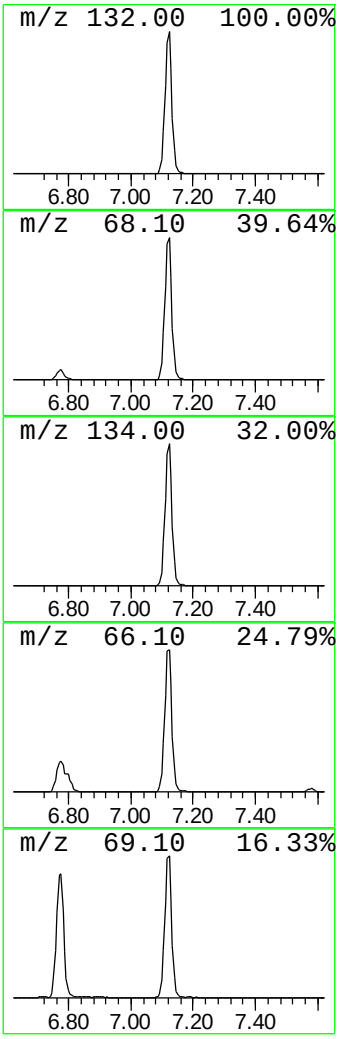
****

Peak Number 1 unknown7.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	40.34 ng	3465310	1,4-Dichlorobenzene-d4	7.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
Data File : BM017912.D
Acq On : 04 Dec 2018 20:59
Operator : JU/SJ
Sample : J5770-15 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : OR-03-112918-B

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

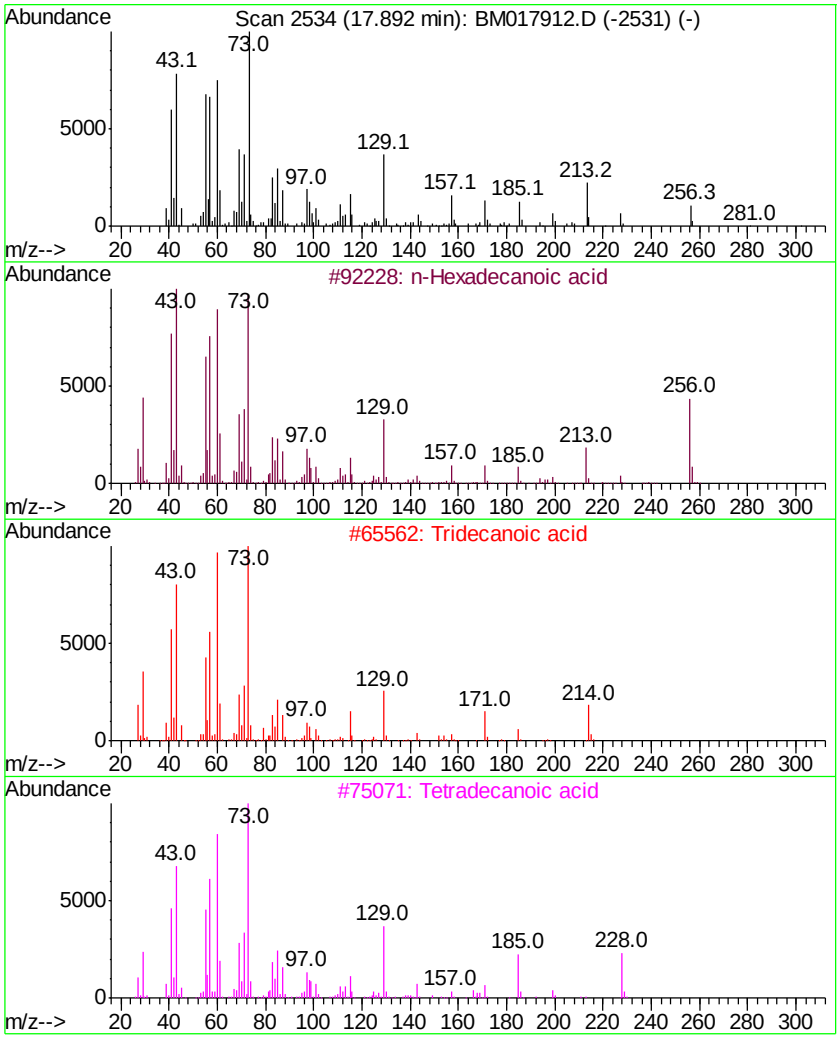
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

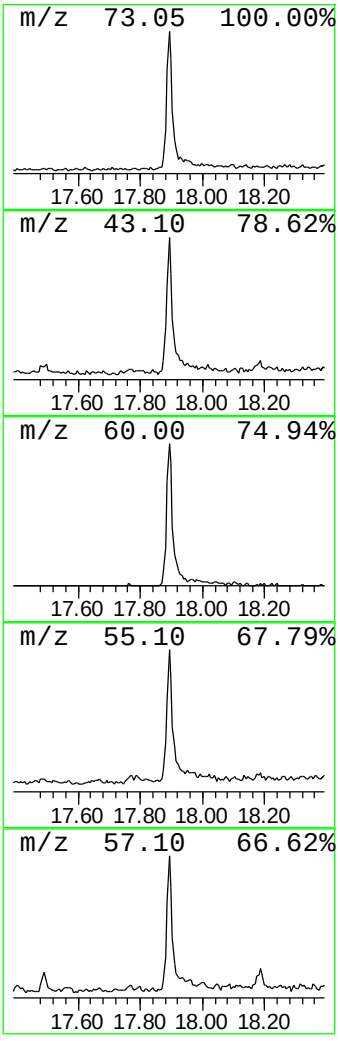
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	5.16 ng	661442	Phenanthrene-d10	16.99

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	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	62
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120518\
Data File : BM017912.D
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Operator : JU/SJ
Sample : J5770-15 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : OR-03-112918-B

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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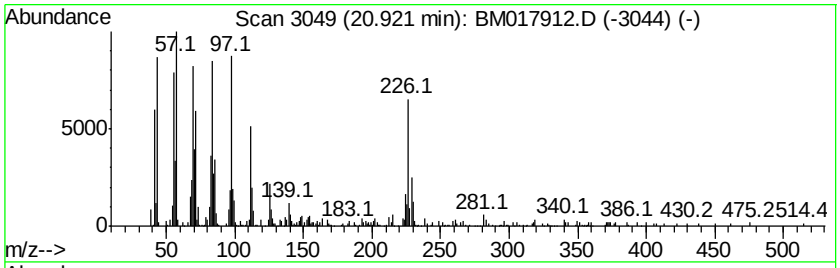
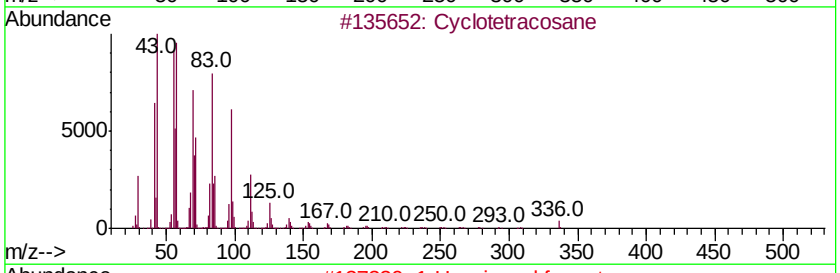
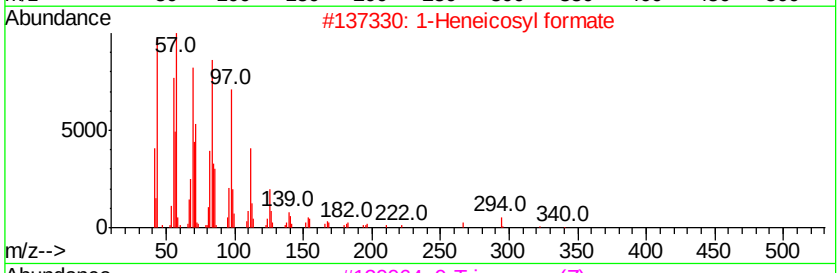
Peak Number 4 Cyclotetracosane Concentration Rank 4

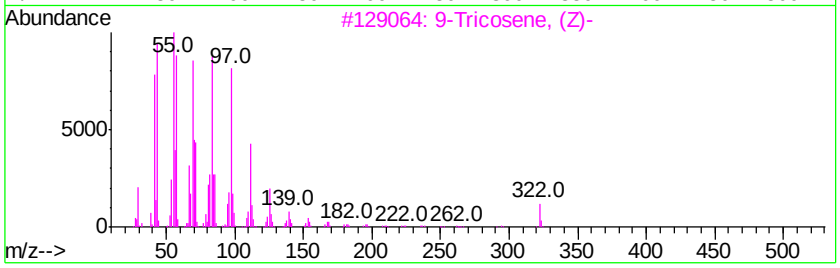
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.92	3.59 ng	602702	Chrysene-d12	21.19

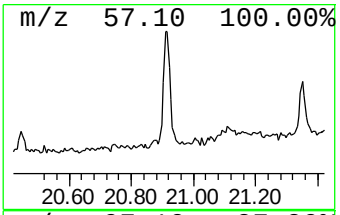
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	96
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	89
5	Cyclopentadecane	210	C15H30	000295-48-7	78

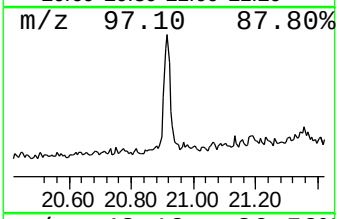


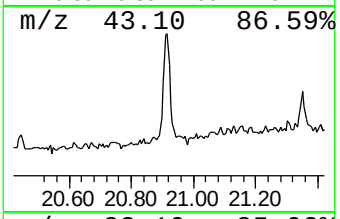


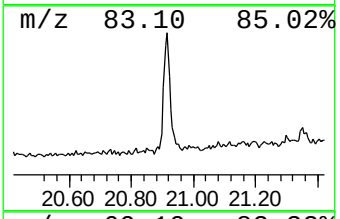


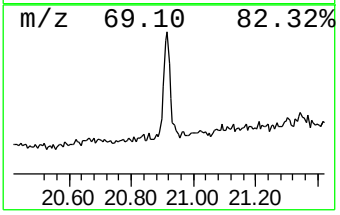












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM120518\
Data File : BM017912.D
Acq On : 04 Dec 2018 20:59
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Instrument : BNA_M
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.12	7.12	40.3	ng	3465310	1	7.58	1718260	20.0
n-Hexadecanoic acid	17.89	5.2	ng	661442	4	16.99	2561910	20.0
Cyclotetracosane	20.92	3.6	ng	602702	5	21.19	3358020	20.0