LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM083019\
Data File : BM022462.D
Acq On : 31 Aug 2019 04:03
Operator : HP/JU
Sample : K4439-02 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-1-(1-3)

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-BM082919.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	5.145	362	367	380	rBB	105299	165954	22.05%	3.128%
2	6.722	630	635	649	rBV	93393	175386	23.30%	3.306%
3	7.057	687	692	702	rBV	119306	188674	25.07%	3.557%
4	7.516	765	770	778	rBB	91227	135452	18.00%	2.553%
5	7.828	818	823	830	rBB	102728	154540	20.53%	2.913%
6	8.698	965	971	986	rBV	55959	106153	14.10%	2.001%
7	10.292	1236	1242	1248	rBV	93260	158315	21.03%	2.984%
8	10.345	1248	1251	1258	rVB2	5518	8544	1.14%	0.161%
9	11.974	1524	1528	1533	rBB	4955	8037	1.07%	0.152%
10	12.786	1660	1666	1677	rBV	157245	227056	30.17%	4.280%
11	13.663	1812	1815	1822	rVB	11959	15829	2.10%	0.298%
12	13.904	1852	1856	1864	rBB	5560	8022	1.07%	0.151%
13	14.180	1898	1903	1912	rBV2	140971	216600	28.78%	4.083%
14	15.698	2156	2161	2169	rBV	161416	229033	30.43%	4.318%
15	15.892	2189	2194	2202	rBV4	7510	18014	2.39%	0.340%
16	16.621	2312	2318	2322	rBV4	6510	12184	1.62%	0.230%
17	16.686	2325	2329	2333	rBV3	8148	12370	1.64%	0.233%
18	16.951	2369	2374	2379	rBV2	212788	298414	39.65%	5.626%
19	16.992	2379	2381	2386	rVB	35827	41758	5.55%	0.787%
20	17.092	2394	2398	2401	rBV2	9001	13055	1.73%	0.246%
21	17.139	2401	2406	2412	rVV2	5151	14879	1.98%	0.280%
22	17.239	2416	2423	2427	rVV4	7198	16222	2.16%	0.306%
23	17.274	2427	2429	2436	rVB4	8513	13246	1.76%	0.250%
24	17.427	2449	2455	2458	rVB4	8857	15989	2.12%	0.301%
25	17.551	2474	2476	2481	rVB2	6940	9164	1.22%	0.173%
26	17.845	2518	2526	2529	rBV2	32695	78147	10.38%	1.473%
27	17.874	2529	2531	2535	rVB	40151	49905	6.63%	0.941%
28	18.015	2550	2555	2559	rBV3	30994	43406	5.77%	0.818%
29	18.056	2559	2562	2568	rVB3	15395	24210	3.22%	0.456%
30	18.115	2568	2572	2575	rBV2	7896	10006	1.33%	0.189%
31	18.156	2575	2579	2583	rBV5	5930	10657	1.42%	0.201%
32	18.227	2587	2591	2595	rVB4	10780	17345	2.30%	0.327%
33	18.339	2604	2610	2616	rBV3	23121	38347	5.09%	0.723%
34	18.580	2645	2651	2656	rVV6	12938	25372	3.37%	0.478%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM083019\
Data File : BM022462.D
Acq On : 31 Aug 2019 04:03
Operator : HP/JU
Sample : K4439-02 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-1-(1-3)

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-BM082919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.633	2656	2660	2664	rVV2	20703	25707	3.42%	0.485%
36	18.674	2664	2667	2670	rVB2	15974	17359	2.31%	0.327%
37	18.756	2676	2681	2686	rBV	51555	80567	10.70%	1.519%
38	18.815	2686	2691	2694	rVV3	12109	19448	2.58%	0.367%
39	18.845	2694	2696	2700	rVB2	16231	17792	2.36%	0.335%
40	18.892	2700	2704	2706	rBV3	14497	17340	2.30%	0.327%
41	19.027	2721	2727	2732	rBV	114696	168437	22.38%	3.175%
42	19.092	2734	2738	2740	rVV	22318	30579	4.06%	0.576%
43	19.139	2741	2746	2749	rVB6	14372	29535	3.92%	0.557%
44	19.297	2771	2773	2778	rBV5	9276	14185	1.88%	0.267%
45	19.362	2780	2784	2785	rBV2	19383	30053	3.99%	0.567%
46	19.392	2785	2789	2797	rVV	120902	175763	23.35%	3.313%
47	19.462	2798	2801	2805	rVB	30024	41188	5.47%	0.776%
48	19.597	2819	2824	2830	rBV	476477	596419	79.24%	11.243%
49	19.709	2839	2843	2845	rBV3	26557	41926	5.57%	0.790%
50	19.856	2866	2868	2869	rBV	12669	7971	1.06%	0.150%
51	20.192	2922	2925	2930	rBV	26035	42018	5.58%	0.792%
52	20.656	3001	3004	3007	rBV	43559	51031	6.78%	0.962%
53	21.168	3085	3091	3095	rBV2	497196	752694	100.00%	14.189%
54	23.356	3458	3463	3469	rBV	325676	584352	77.63%	11.016%

Sum of corrected areas: 5304649

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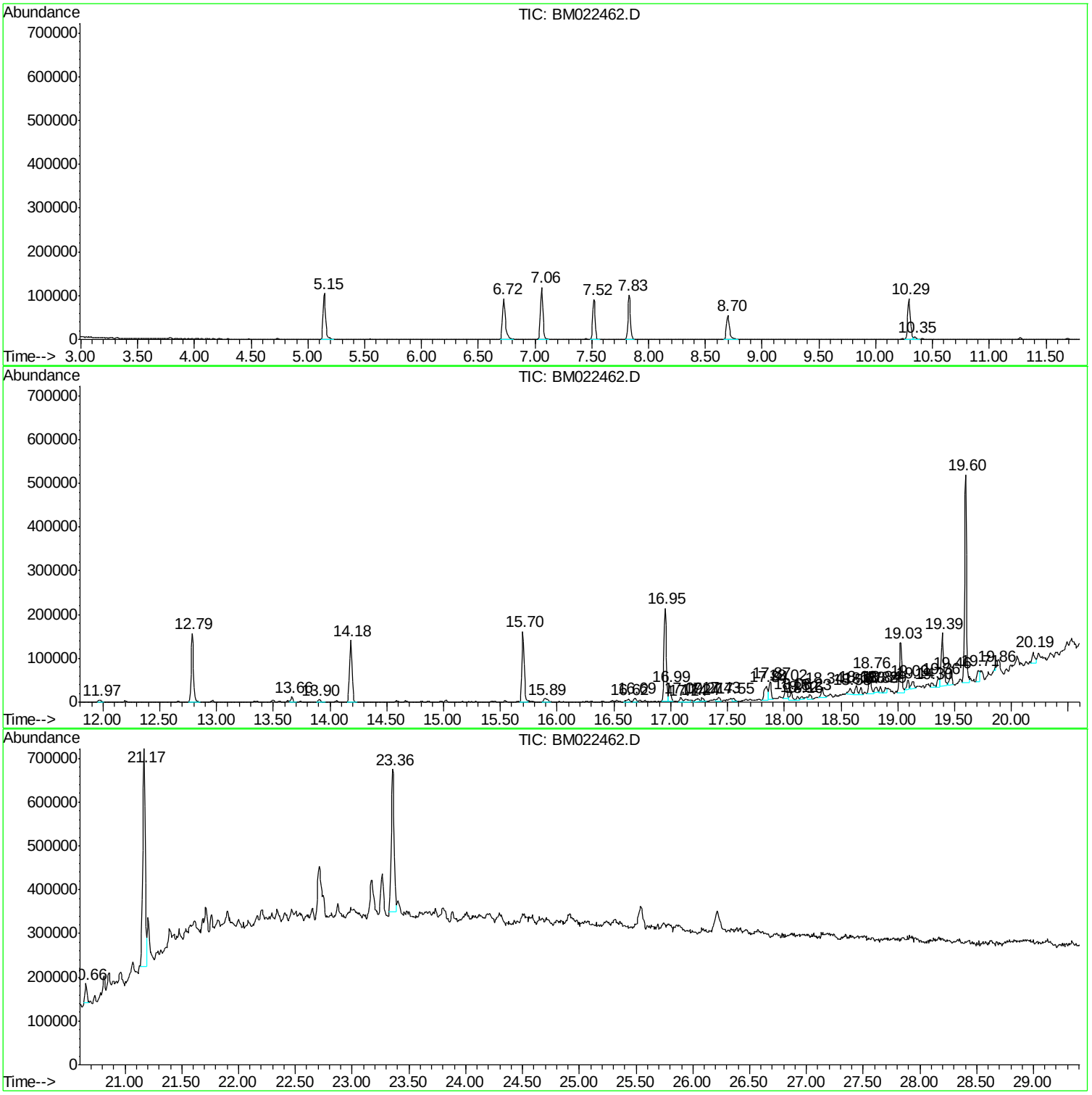
Data File : BM022462.D
Acq On : 31 Aug 2019 04:03
Operator : HP/JU
Sample : K4439-02 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-1-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM083019\
Data File : BM022462.D
Acq On : 31 Aug 2019 04:03
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-1-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
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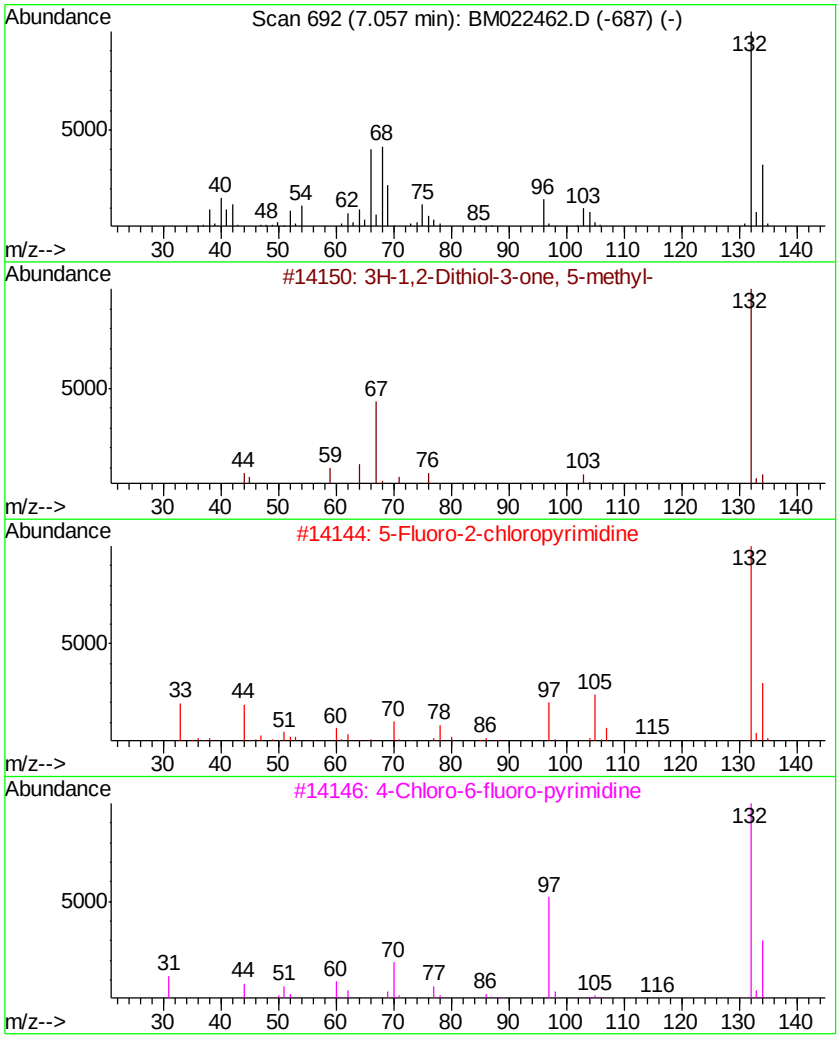
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

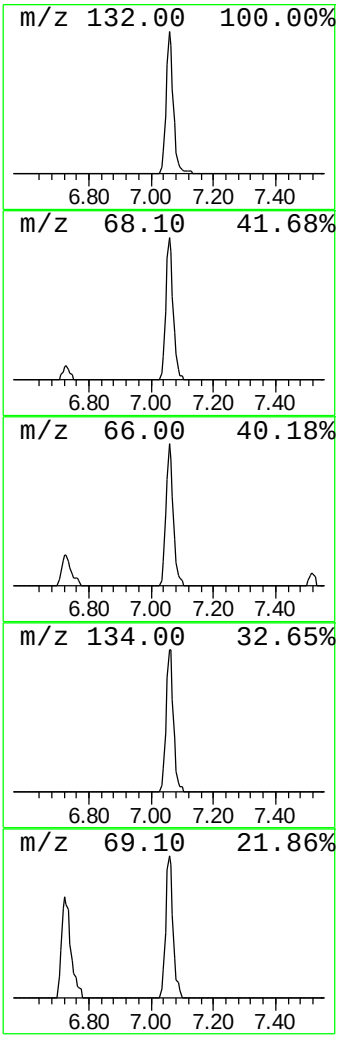
****

Peak Number 1 unknown7.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	27.86 ng	188674	1,4-Dichlorobenzene-d4	7.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM083019\
Data File : BM022462.D
Acq On : 31 Aug 2019 04:03
Operator : HP/JU
Sample : K4439-02 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-1-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.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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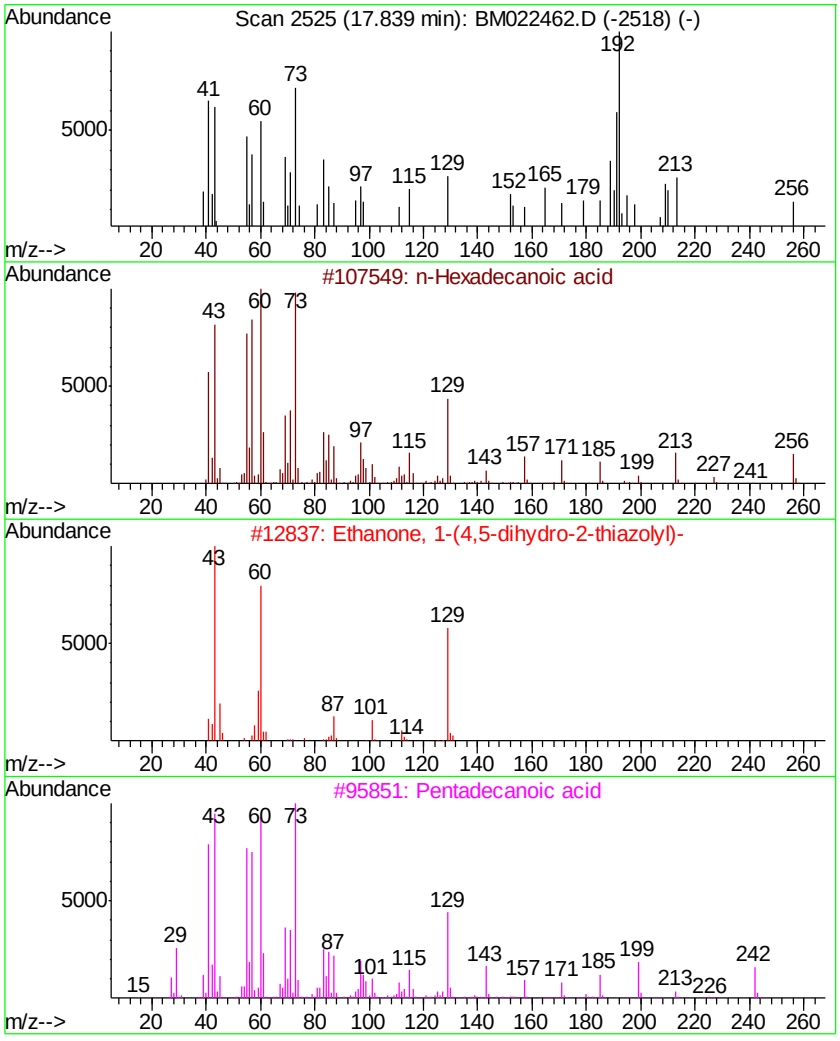
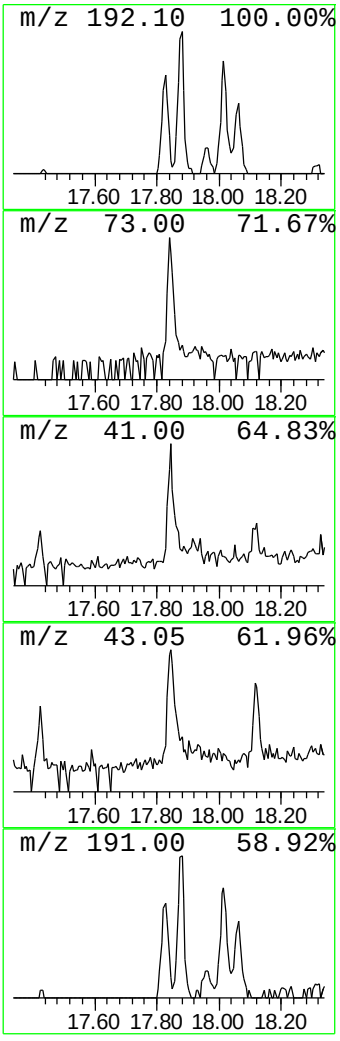
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.84	5.24 ng	78147	Phenanthrene-d10	16.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	30
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	30
4	Tridecanoic acid	214	C13H26O2	000638-53-9	27
5	Dodecanoic acid	200	C12H24O2	000143-07-7	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM083019\
Data File : BM022462.D
Acq On : 31 Aug 2019 04:03
Operator : HP/JU
Sample : K4439-02 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-1-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

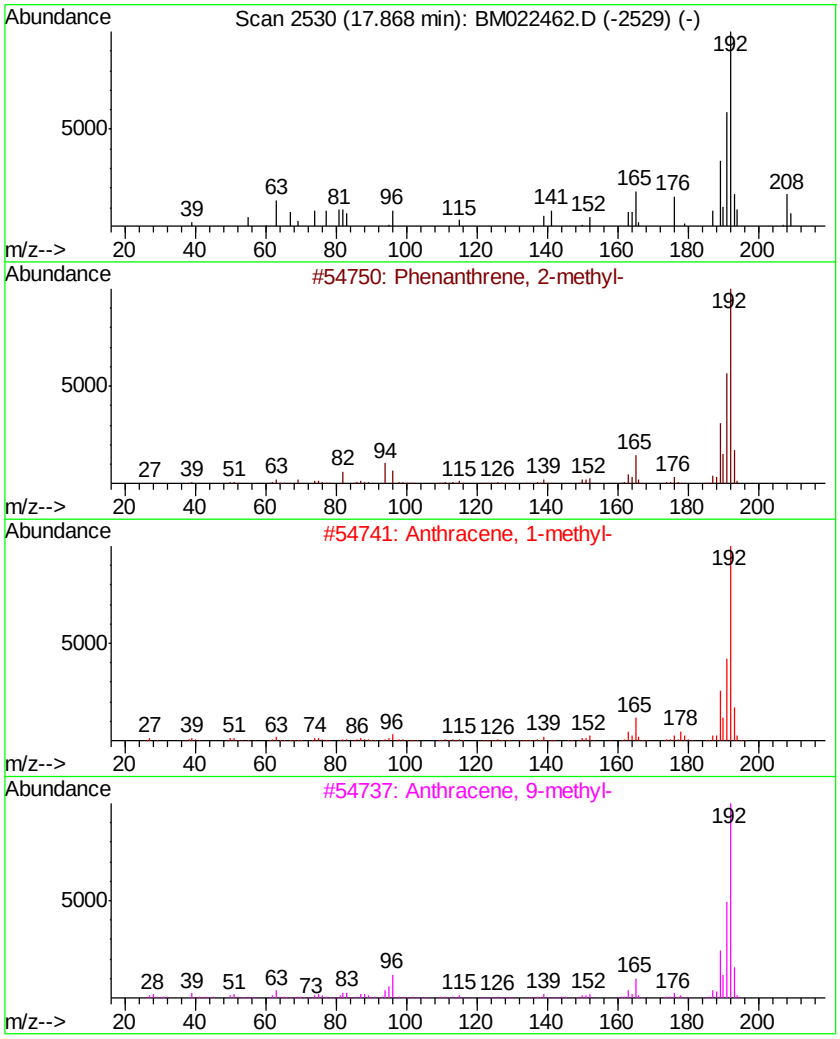
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

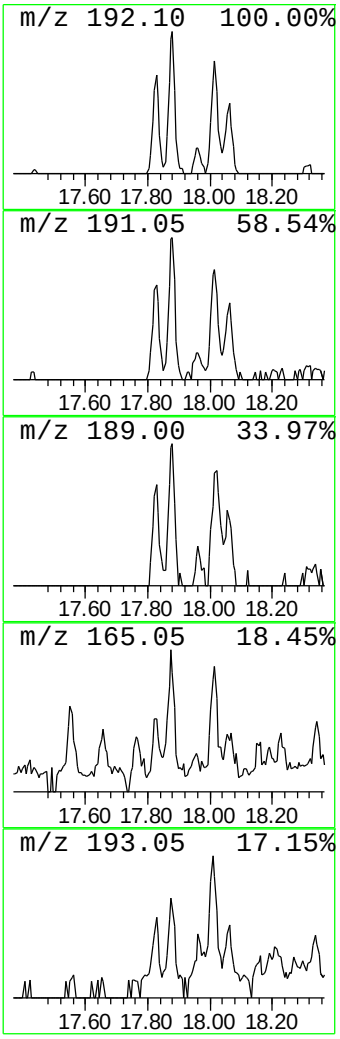
****

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.87	3.34 ng	49905	Phenanthrene-d10	16.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	81
4	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	74
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	70





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM083019\
Data File : BM022462.D
Acq On : 31 Aug 2019 04:03
Operator : HP/JU
Sample : K4439-02 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-1-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

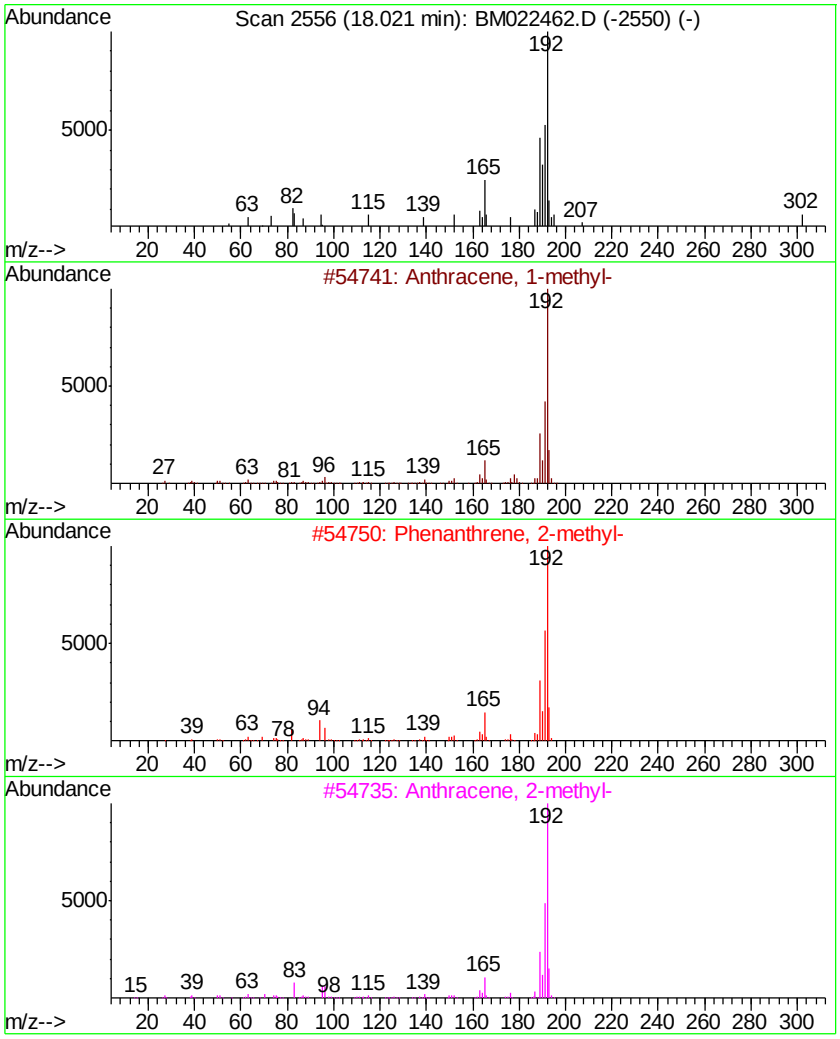
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

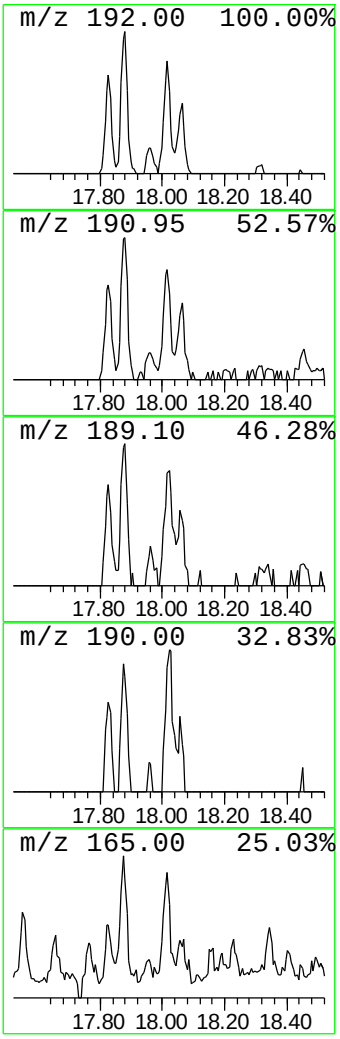
****

Peak Number 5 Anthracene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.02	2.91 ng	43406	Phenanthrene-d10	16.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	90





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Misc :
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Instrument : BNA_M
ClientSampleId : S-1-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

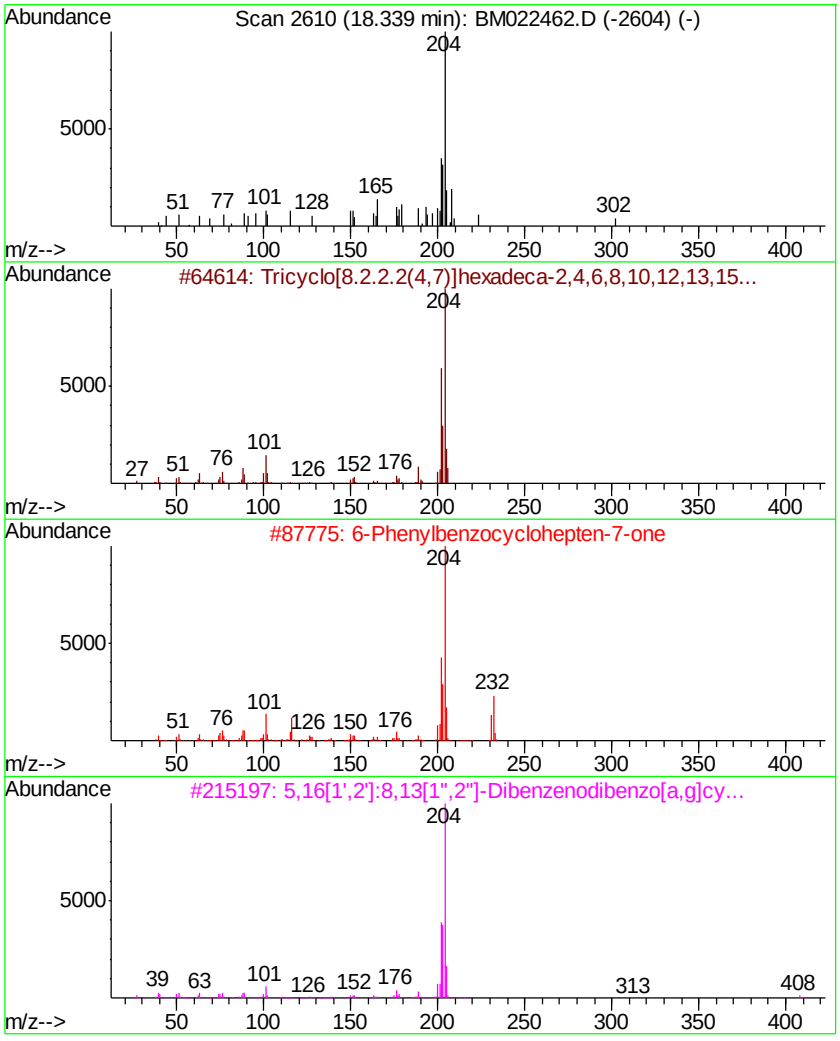
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

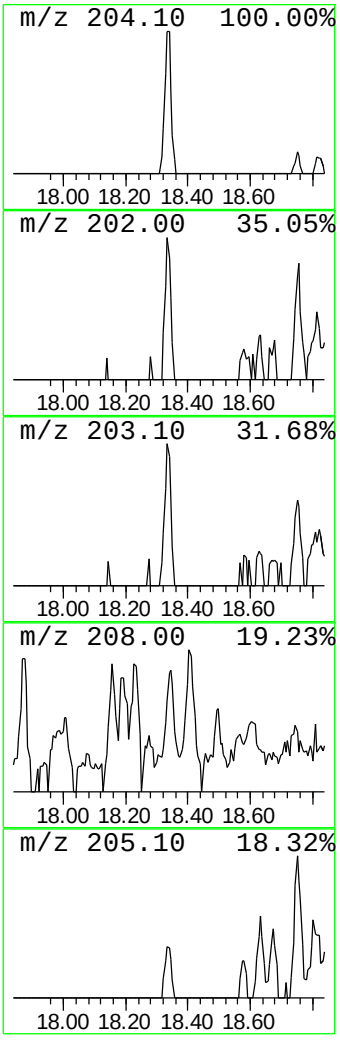
****

Peak Number 6 Tricyclo[8.2.2.2(4,7)]hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	2.57 ng	38347	Phenanthrene-d10	16.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	64
2	6-Phenylbenzocyclohepten-7-one	232	C17H12O	093327-56-1	59
3	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	59
4	9,10-di(Chloromethyl)anthracene	274	C16H12Cl2	010387-13-0	59
5	9,10-Bis(bromomethyl)anthracene	362	C16H12Br2	034373-96-1	59





Library Search Compound Report

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Misc :
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Instrument : BNA_M
ClientSampleId : S-1-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

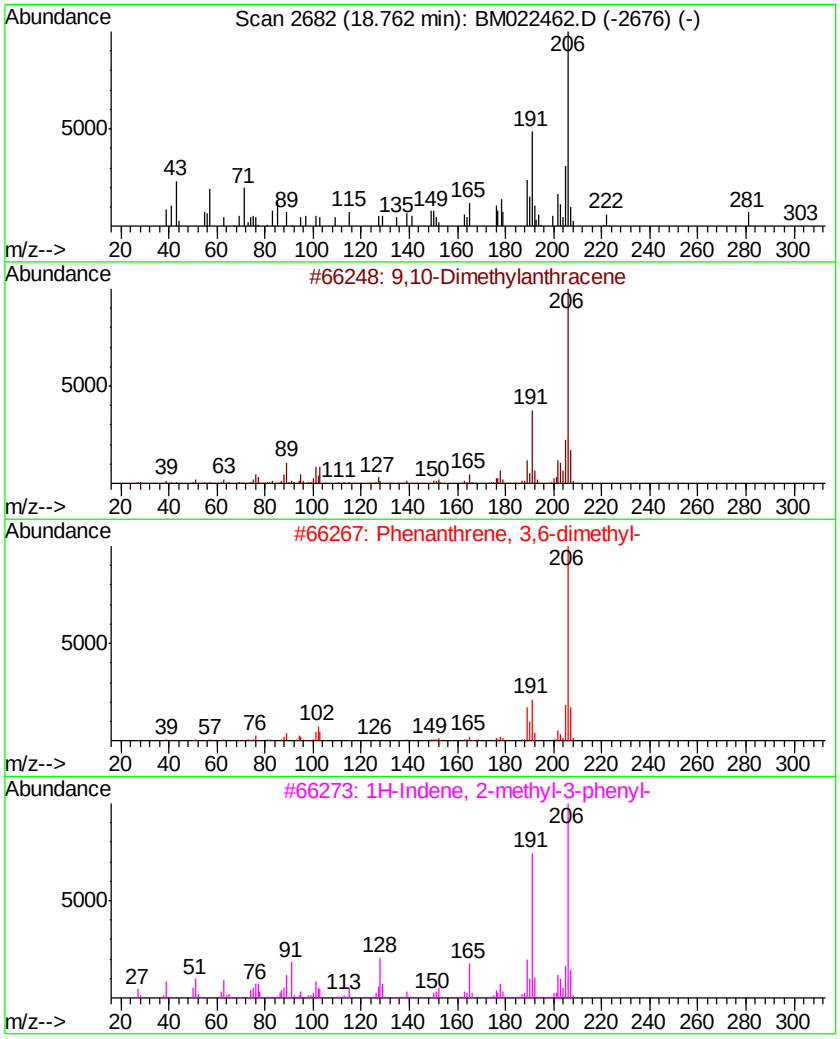
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

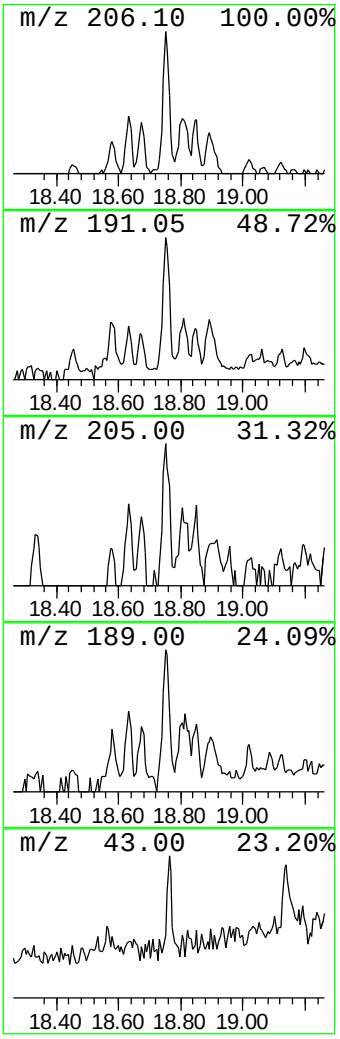
****

Peak Number 7 9,10-Dimethylanthracene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.76	5.40 ng	80567	Phenanthrene-d10	16.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	91
2	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	87
3	1H-Indene, 2-methyl-3-phenyl-	206	C16H14	035099-60-6	86
4	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	83
5	3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM083019\
Data File : BM022462.D
Acq On : 31 Aug 2019 04:03
Operator : HP/JU
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Misc :
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Instrument : BNA_M
ClientSampleId : S-1-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
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
unknown7.06	7.06	27.9	ng	188674	1	7.52	135452	20.0
n-Hexadecanoic acid	17.84	5.2	ng	78147	4	16.95	298414	20.0
Phenanthrene, 2-m...	17.87	3.3	ng	49905	4	16.95	298414	20.0
Anthracene, 1-met...	18.02	2.9	ng	43406	4	16.95	298414	20.0
Tricyclo[8.2.2.2(...	18.34	2.6	ng	38347	4	16.95	298414	20.0
9,10-Dimethylanth...	18.76	5.4	ng	80567	4	16.95	298414	20.0