LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097644.D
Acq On : 12 Aug 2017 20:21
Operator : SJ/JU
Sample : I4683-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAPTAINSCOVE-WC-001

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:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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	1.881	31	33	40	rVB5	8582	14388	1.51%	0.150%
2	4.734	515	518	529	rBV2	11864	33215	3.50%	0.346%
3	5.428	633	636	657	rBV	160417	496615	52.28%	5.171%
4	7.069	912	915	928	rBV	197162	488450	51.42%	5.086%
5	7.169	928	932	958	rVB	321327	706670	74.40%	7.358%
6	7.498	984	988	1005	rBV	527781	758922	79.90%	7.902%
7	7.739	1025	1029	1047	rBV	257261	394213	41.50%	4.105%
8	8.416	1141	1144	1169	rBV	131880	312725	32.92%	3.256%
9	9.527	1329	1333	1346	rBV	647301	890912	93.79%	9.276%
10	11.304	1630	1635	1650	rBV	372115	474630	49.97%	4.942%
11	11.815	1717	1722	1726	rBV2	37116	40237	4.24%	0.419%
12	11.998	1749	1753	1760	rBV	50798	67619	7.12%	0.704%
13	12.351	1808	1813	1822	rBV2	686512	949856	100.00%	9.890%
14	12.421	1822	1825	1830	rVV3	13962	16361	1.72%	0.170%
15	12.474	1830	1834	1838	rVB	8722	10115	1.06%	0.105%
16	13.204	1954	1958	1964	rVB3	7499	10644	1.12%	0.111%
17	13.651	2030	2034	2052	rVB2	117458	191158	20.12%	1.990%
18	13.974	2085	2089	2096	rBV	8687	14641	1.54%	0.152%
19	14.745	2216	2220	2225	rVV2	527429	695444	73.22%	7.241%
20	14.786	2225	2227	2234	rVB	42577	59961	6.31%	0.624%
21	14.892	2241	2245	2249	rBV2	8625	10076	1.06%	0.105%
22	15.274	2307	2310	2317	rBV3	7566	13237	1.39%	0.138%
23	15.745	2386	2390	2397	rVB3	8216	12483	1.31%	0.130%
24	16.462	2509	2512	2519	rBV4	9260	18613	1.96%	0.194%
25	16.556	2524	2528	2534	rVB	75182	92499	9.74%	0.963%
26	16.645	2540	2543	2547	rBV	23720	27029	2.85%	0.281%
27	16.856	2575	2579	2585	rBV	84842	98192	10.34%	1.022%
28	17.097	2616	2620	2627	rVB	269006	289815	30.51%	3.018%
29	17.333	2656	2660	2665	rVB4	7786	12042	1.27%	0.125%
30	17.462	2678	2682	2687	rBV4	10153	19693	2.07%	0.205%
31	18.362	2830	2835	2843	rBV3	29574	55138	5.80%	0.574%
32	18.444	2843	2849	2854	rBV	500226	640767	67.46%	6.672%
33	18.515	2859	2861	2865	rVB2	21066	20690	2.18%	0.215%
34	18.574	2865	2871	2875	rBV6	11665	18324	1.93%	0.191%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097644.D
Acq On : 12 Aug 2017 20:21
Operator : SJ/JU
Sample : I4683-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAPTAINSCOVE-WC-001

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:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.750	2897	2901	2903	rBV4	5902	10415	1.10%	0.108%
36	18.915	2926	2929	2933	rBV4	18248	18611	1.96%	0.194%
37	19.150	2966	2969	2977	rVB4	29345	54620	5.75%	0.569%
38	19.515	3028	3031	3034	rBV5	17148	18890	1.99%	0.197%
39	19.586	3035	3043	3048	rVB	82592	114012	12.00%	1.187%
40	19.668	3054	3057	3062	rBV	74844	95105	10.01%	0.990%
41	19.715	3062	3065	3068	rVV	45286	57175	6.02%	0.595%
42	19.827	3082	3084	3088	rBV3	8961	11563	1.22%	0.120%
43	19.874	3088	3092	3095	rBV	94860	109220	11.50%	1.137%
44	19.903	3095	3097	3104	rVB4	37051	60818	6.40%	0.633%
45	20.009	3112	3115	3120	rBV	26408	31888	3.36%	0.332%
46	20.062	3121	3124	3128	rVV	43491	47866	5.04%	0.498%
47	20.115	3128	3133	3142	rVB	412673	547261	57.62%	5.698%
48	20.215	3147	3150	3153	rVB3	24177	28729	3.02%	0.299%
49	20.374	3173	3177	3185	rVB2	63096	87467	9.21%	0.911%
50	20.568	3205	3210	3215	rVB	171846	226338	23.83%	2.357%
51	20.956	3273	3276	3280	rVB3	25392	31001	3.26%	0.323%
52	21.180	3310	3314	3318	rBV2	36522	52567	5.53%	0.547%
53	21.297	3333	3334	3336	rBV2	17196	12743	1.34%	0.133%
54	23.421	3694	3695	3698	rBV3	14405	18983	2.00%	0.198%
55	23.762	3751	3753	3754	rBV	16470	13387	1.41%	0.139%

Sum of corrected areas: 9604033

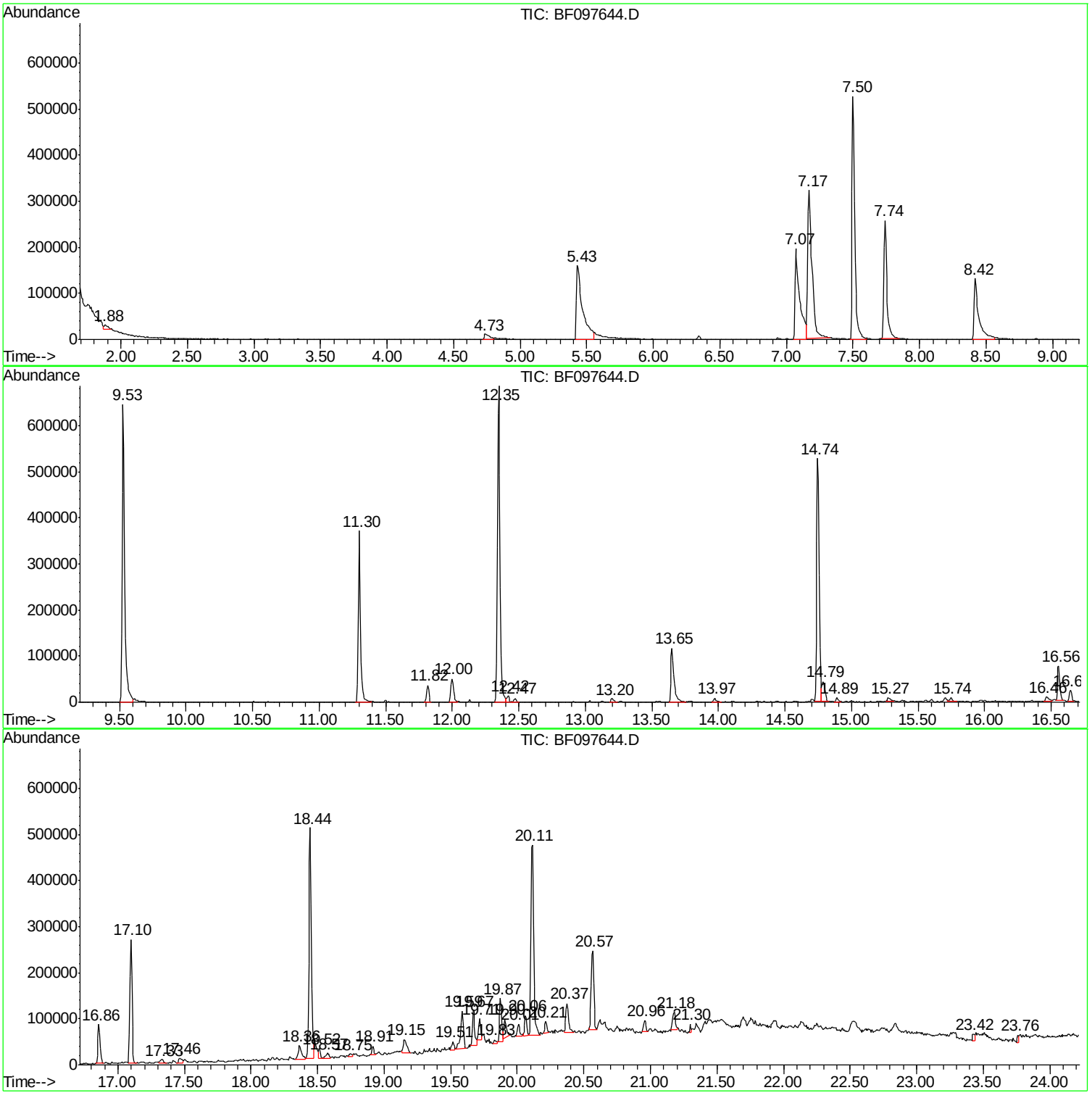
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097644.D
Acq On : 12 Aug 2017 20:21
Operator : SJ/JU
Sample : I4683-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAPTAINSCOVE-WC-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097644.D
Acq On : 12 Aug 2017 20:21
Operator : SJ/JU
Sample : I4683-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAPTAINSCOVE-WC-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

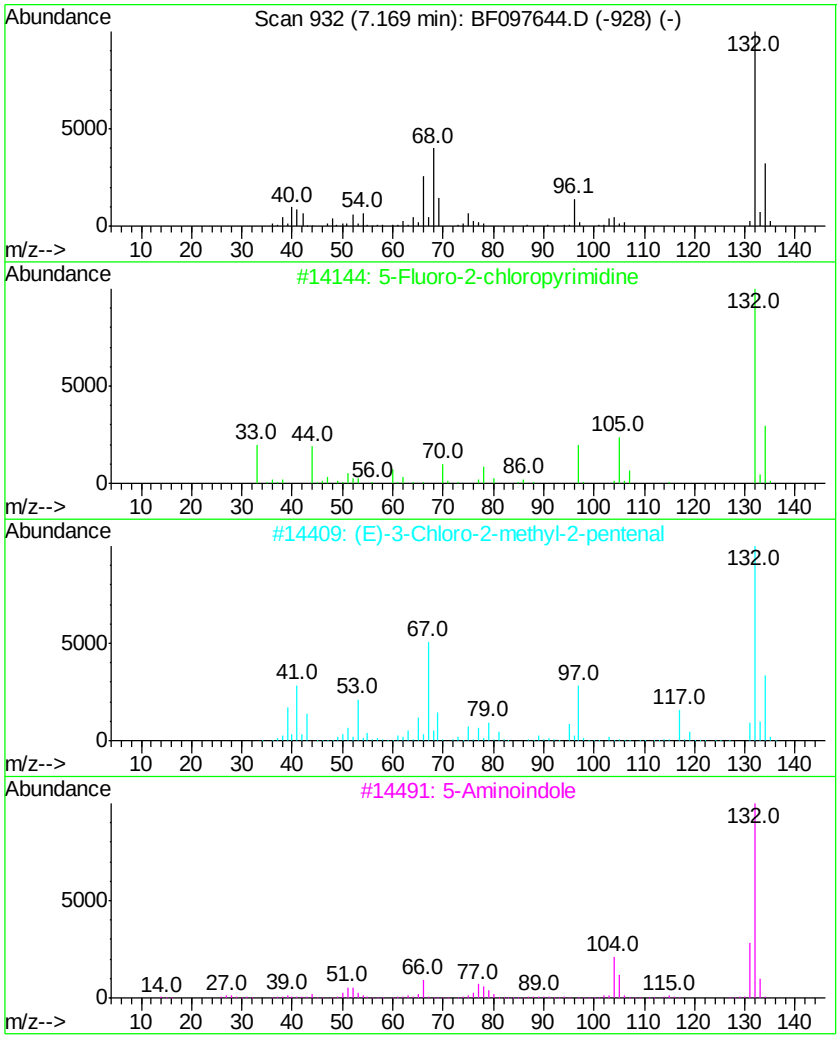
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

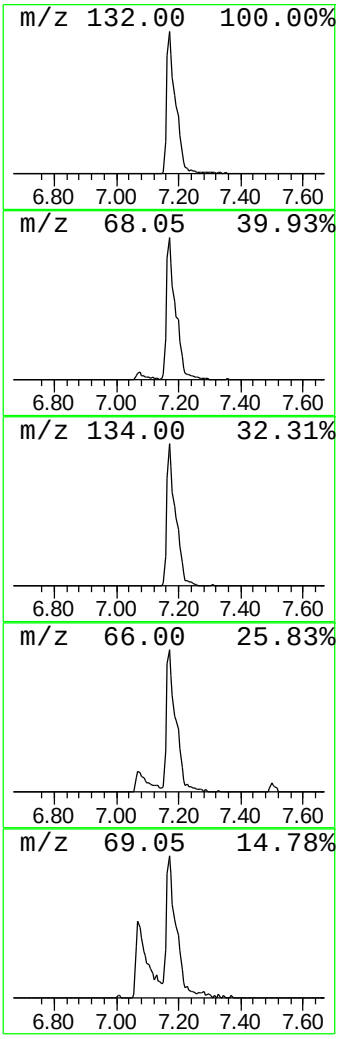
****

Peak Number 1 unknown7.17 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.17	18.62 ng	706670	1,4-Dichlorobenzene-d4	7.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Amphetaminil	250	C17H18N2	017590-01-1	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097644.D
Acq On : 12 Aug 2017 20:21
Operator : SJ/JU
Sample : I4683-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAPTAINSCOVE-WC-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

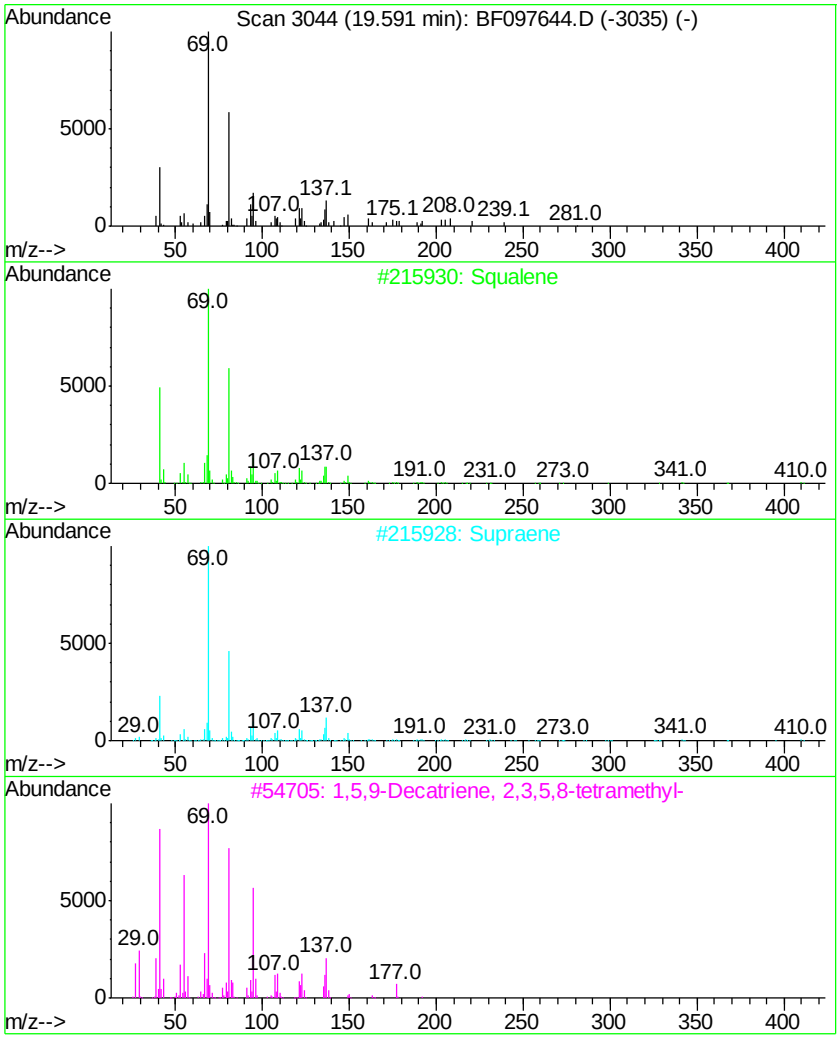
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

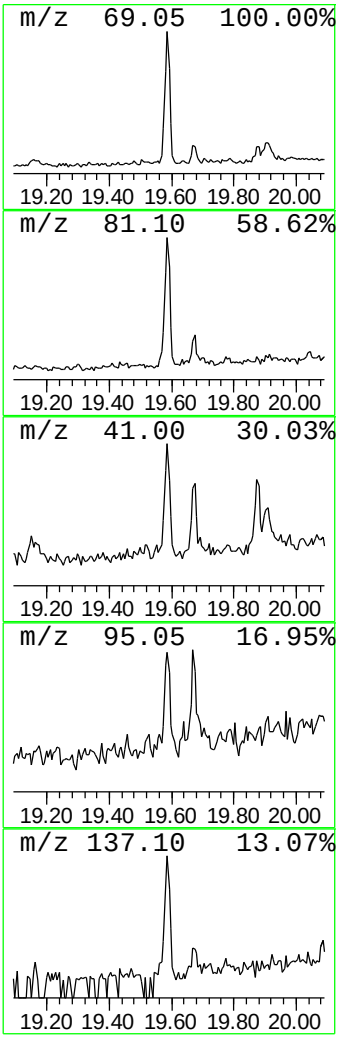
****

Peak Number 3 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.59	4.17 ng	114012	Perylene-d12	20.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	87
3	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	83
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5	trans-Farnesol	222	C15H26O	000106-28-5	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097644.D
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Operator : SJ/JU
Sample : I4683-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAPTAINSCOVE-WC-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

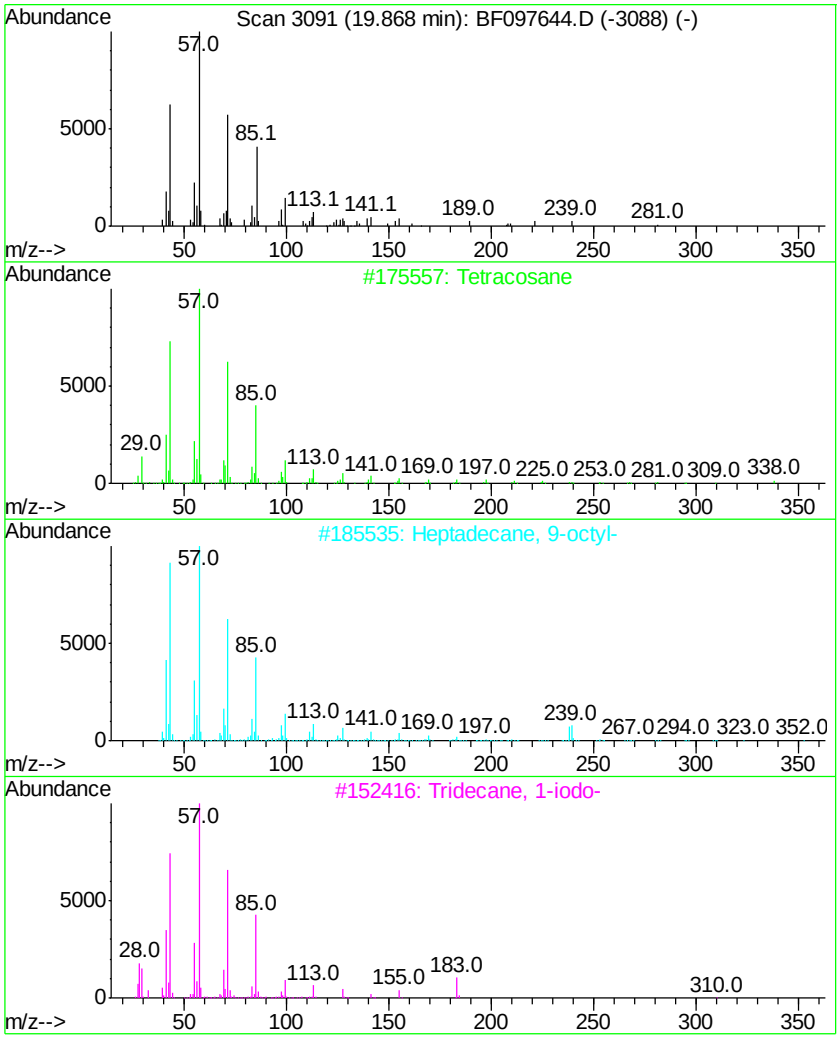
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

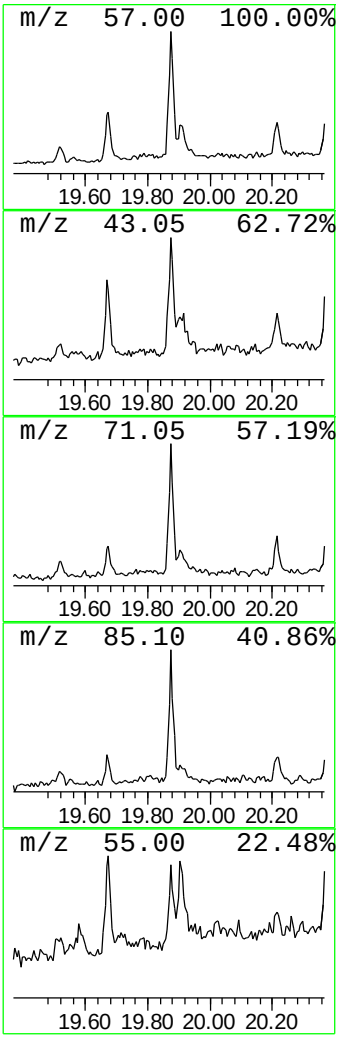
****

Peak Number 4 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.87	3.99 ng	109220	Perylene-d12	20.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5	Heptadecane	240	C17H36	000629-78-7	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
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Acq On : 12 Aug 2017 20:21
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Sample : I4683-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAPTAINSCOVE-WC-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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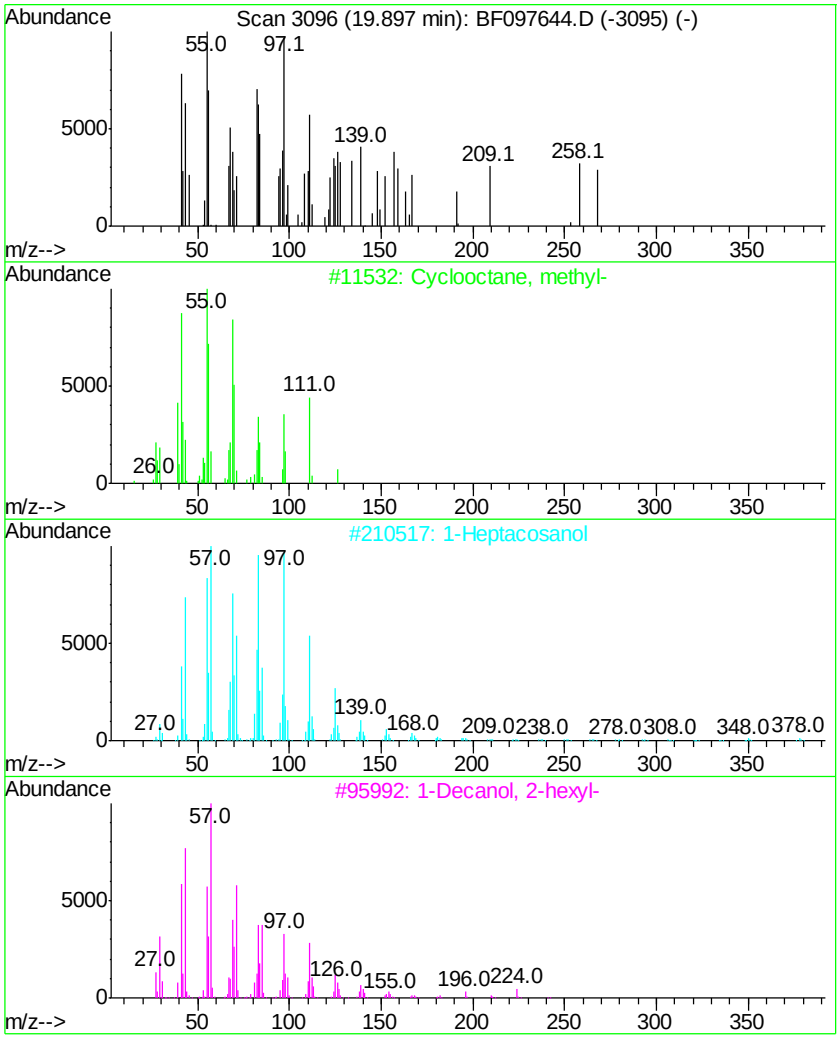
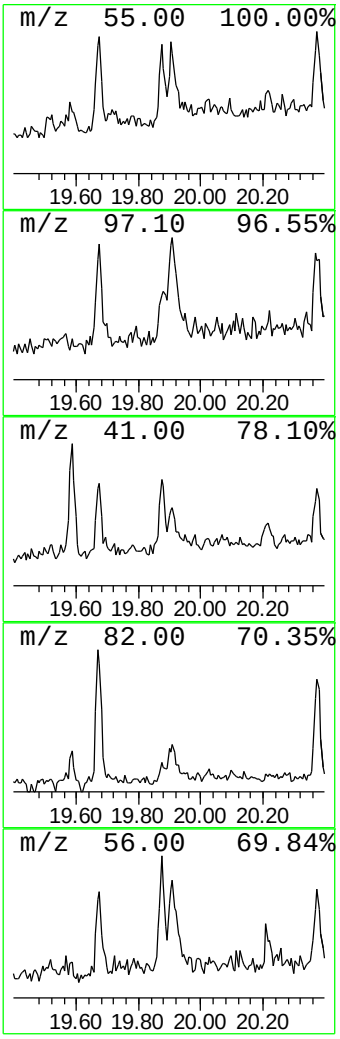
Peak Number 5 unknown19.90 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	2.22 ng	60818	Perylene-d12	20.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane, methyl-	126	C9H18	001502-38-1	49
2	1-Heptacosanol	396	C27H56O	002004-39-9	38
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	38
4	2,2-Dimethylpropanoic acid, unde...	254	C16H30O2	1000299-33-7	35
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	27





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Misc :
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Instrument : BNA_F
ClientSampleId : CAPTAINSCOVE-WC-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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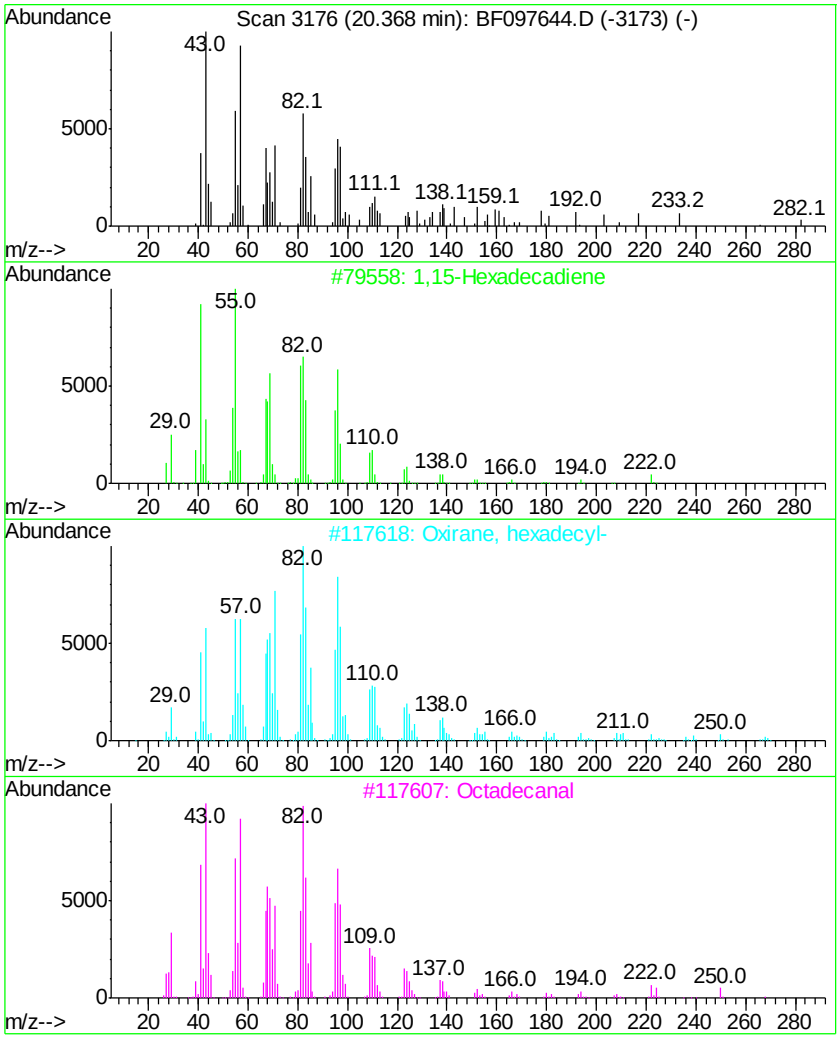
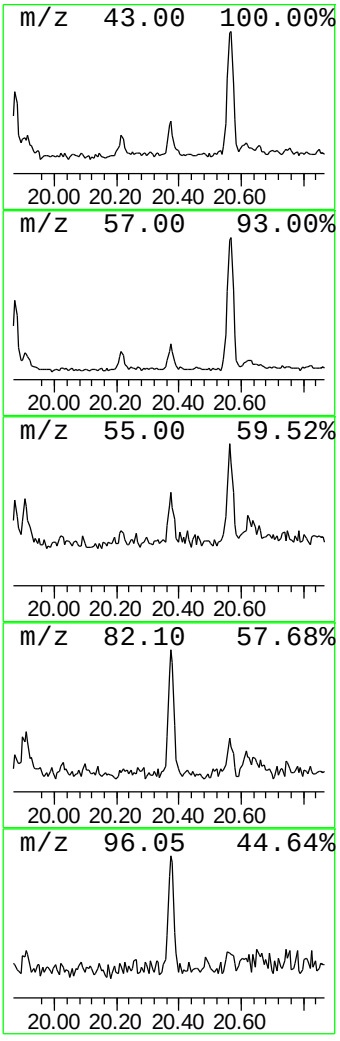
Peak Number 6 1,15-Hexadecadiene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.37	3.20 ng	87467	Perylene-d12	20.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,15-Hexadecadiene	222	C16H30	021964-51-2	87
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	86
3	Octadecanal	268	C18H36O	000638-66-4	64
4	1,19-Eicosadiene	278	C20H38	014811-95-1	58
5	E-8-Hexadecen-1-ol acetate	282	C18H34O2	1000131-01-1	55





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
Data File : BF097644.D
Acq On : 12 Aug 2017 20:21
Operator : SJ/JU
Sample : I4683-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAPTAINSCOVE-WC-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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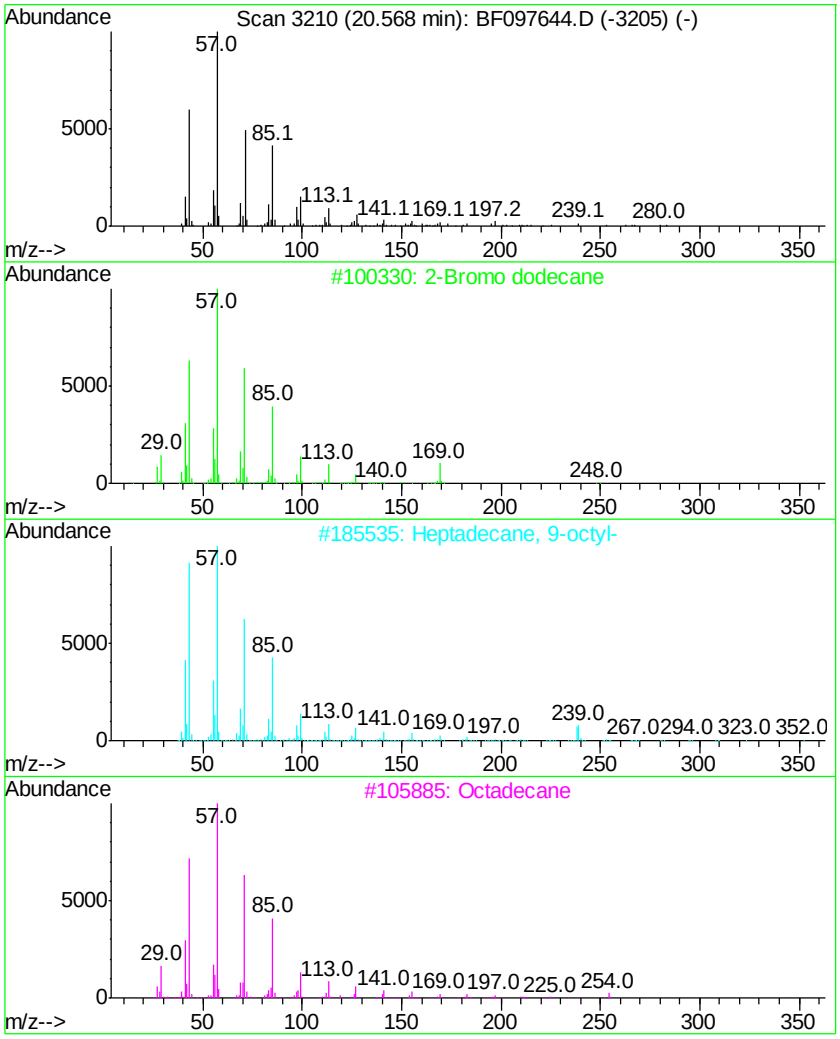
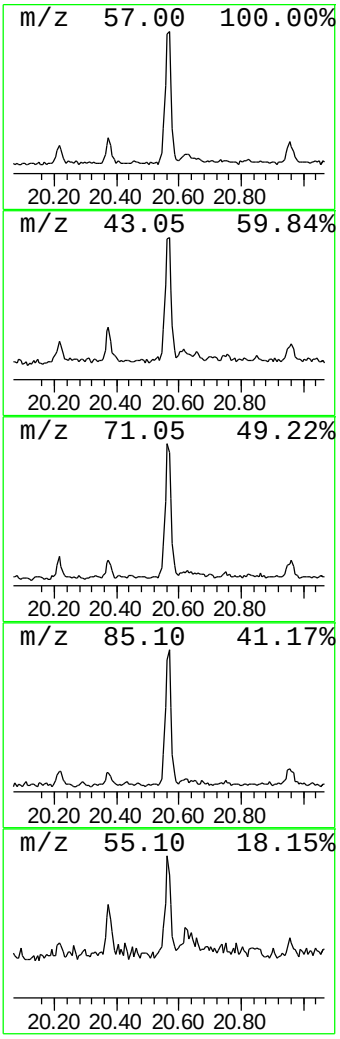
Peak Number 7 2-Bromo dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.57	8.27 ng	226338	Perylene-d12	20.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
3	Octadecane	254	C18H38	000593-45-3	83
4	Heneicosane	296	C21H44	000629-94-7	80
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097644.D
Acq On : 12 Aug 2017 20:21
Operator : SJ/JU
Sample : I4683-01 5X
Misc :
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Instrument : BNA_F
ClientSampleId : CAPTAINSCOVE-WC-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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
unknown7.17	7.17	18.6	ng	706670	1	7.50	758922	20.0
Squalene	19.59	4.2	ng	114012	6	20.11	547261	20.0
Tetracosane	19.87	4.0	ng	109220	6	20.11	547261	20.0
unknown19.90	19.90	2.2	ng	60818	6	20.11	547261	20.0
1,15-Hexadecadiene	20.37	3.2	ng	87467	6	20.11	547261	20.0
2-Bromo dodecane	20.57	8.3	ng	226338	6	20.11	547261	20.0