LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117710.D
Acq On : 7 Nov 2019 17:46
Operator : JU
Sample : K5723-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7-C

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_F\METHODS\8270-BF110619.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	2.246	21	27	41	rVB	1386720	1964824	27.81%	2.736%
2	3.469	231	235	248	rBV	49856	100901	1.43%	0.140%
3	5.151	516	521	530	rVB	1093988	1384351	19.60%	1.927%
4	5.545	583	588	592	rBV	5673399	6031167	85.37%	8.397%
5	6.551	753	759	763	rBV	6163919	6486710	91.82%	9.032%
6	6.698	780	784	788	rBV	6427668	6494368	91.93%	9.042%
7	6.934	820	824	827	rBV	2478372	1914323	27.10%	2.665%
8	7.092	847	851	854	rVB	5850267	5101157	72.21%	7.102%
9	7.492	914	919	922	rBV	4335236	3987908	56.45%	5.552%
10	8.222	1037	1043	1046	rBV	2839242	2564879	36.31%	3.571%
11	9.298	1221	1226	1229	rBV	8037091	7064497	100.00%	9.836%
12	9.686	1289	1292	1296	rVB	1100026	864137	12.23%	1.203%
13	9.980	1336	1342	1345	rBV	3542729	2931596	41.50%	4.082%
14	10.769	1471	1476	1479	rBV	5167100	4532204	64.15%	6.310%
15	10.869	1489	1493	1494	rBV	111415	94171	1.33%	0.131%
16	10.898	1494	1498	1504	rVB3	126859	186172	2.64%	0.259%
17	11.339	1566	1573	1576	rBV4	66450	111706	1.58%	0.156%
18	11.474	1592	1596	1598	rBV	3183804	2928004	41.45%	4.077%
19	11.492	1598	1599	1602	rVV	290282	199138	2.82%	0.277%
20	11.539	1602	1607	1610	rVB3	188246	200015	2.83%	0.278%
21	11.692	1629	1633	1636	rBV	106410	99970	1.42%	0.139%
22	11.974	1678	1681	1682	rBV	107668	97236	1.38%	0.135%
23	11.992	1682	1684	1688	rVB2	526544	535595	7.58%	0.746%
24	12.080	1696	1699	1702	rBV2	103120	103662	1.47%	0.144%
25	12.169	1709	1714	1718	rBV2	86934	103817	1.47%	0.145%
26	12.521	1768	1774	1777	rBV2	96658	107887	1.53%	0.150%
27	12.563	1777	1781	1783	rBV2	99951	105079	1.49%	0.146%
28	12.686	1799	1802	1808	rBV	483098	439192	6.22%	0.611%
29	12.780	1815	1818	1821	rBV	141926	131973	1.87%	0.184%
30	12.916	1835	1841	1843	rBV	406778	375031	5.31%	0.522%
31	13.063	1861	1866	1869	rBV	7288519	6471074	91.60%	9.010%
32	13.133	1872	1878	1882	rBV3	53818	101986	1.44%	0.142%
33	13.639	1958	1964	1971	rBV5	67978	110541	1.56%	0.154%
34	13.957	2014	2018	2026	rBV	543921	577515	8.17%	0.804%

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Integrator: RTE
Smoothing : ON Filtering: 5
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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.115	2040	2045	2048	rBV	2485128	2368295	33.52%	3.297%
36	14.139	2048	2049	2057	rVB	196502	171466	2.43%	0.239%
37	14.280	2070	2073	2079	rVB2	105795	124352	1.76%	0.173%
38	14.592	2120	2126	2130	rBV2	164887	204487	2.89%	0.285%
39	14.910	2177	2180	2184	rBV	138581	148715	2.11%	0.207%
40	14.992	2190	2194	2201	rBV	450123	464065	6.57%	0.646%
41	15.174	2221	2225	2229	rBV	181751	285656	4.04%	0.398%
42	15.268	2237	2241	2243	rBV2	126448	157772	2.23%	0.220%
43	15.492	2275	2279	2286	rVB	116670	156561	2.22%	0.218%
44	15.557	2286	2290	2295	rVB	132141	157819	2.23%	0.220%
45	15.627	2296	2302	2306	rVV	1847286	2331953	33.01%	3.247%
46	15.668	2306	2309	2318	rVB3	134745	202467	2.87%	0.282%
47	16.133	2383	2388	2392	rBV2	95924	165048	2.34%	0.230%
48	16.674	2474	2480	2488	rBV4	50508	115580	1.64%	0.161%
49	17.145	2555	2560	2569	rVB2	72453	148030	2.10%	0.206%
50	17.603	2634	2638	2649	rVB	54249	118041	1.67%	0.164%

Sum of corrected areas: 71823093

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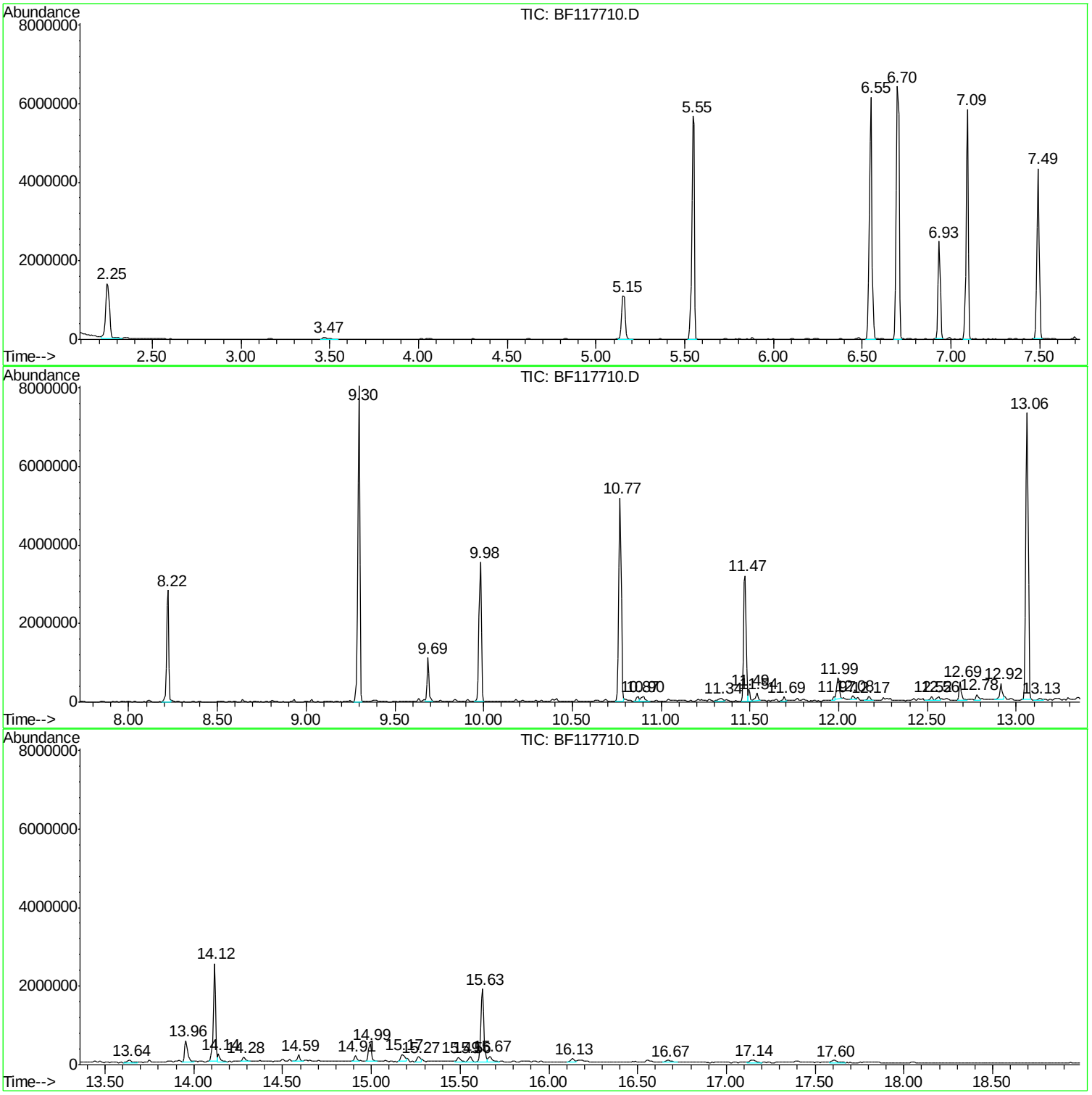
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF117710.D
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Operator : JU
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Instrument : BNA_F
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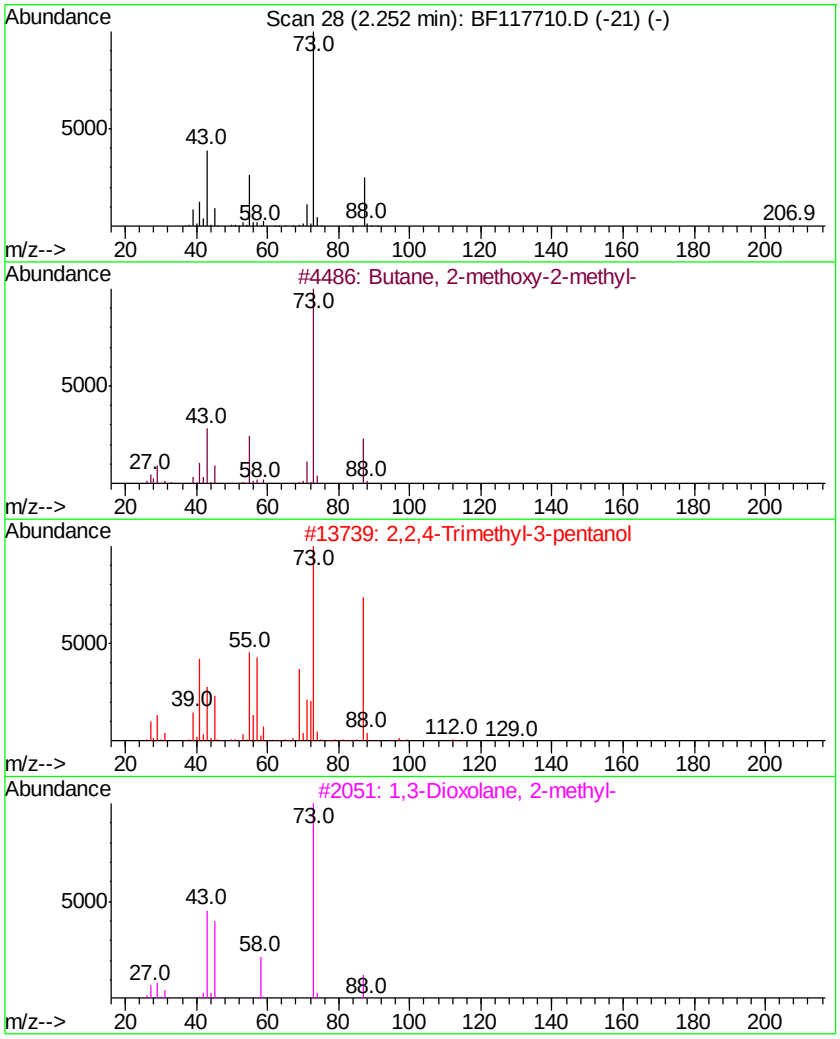
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

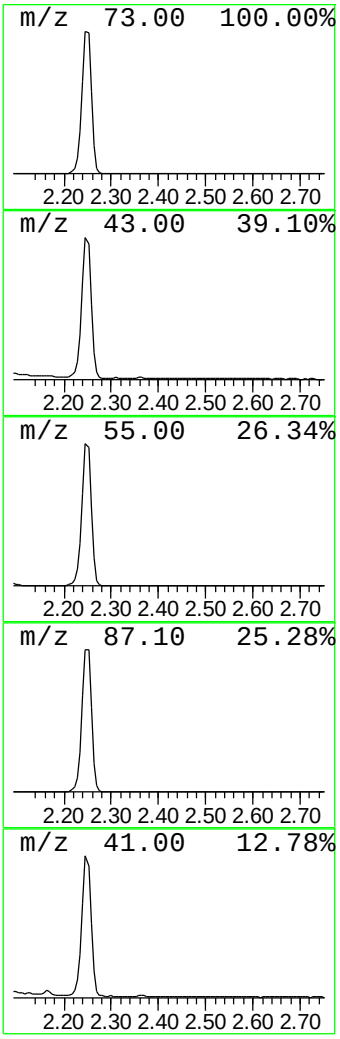
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	20.53 ng	1964820	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

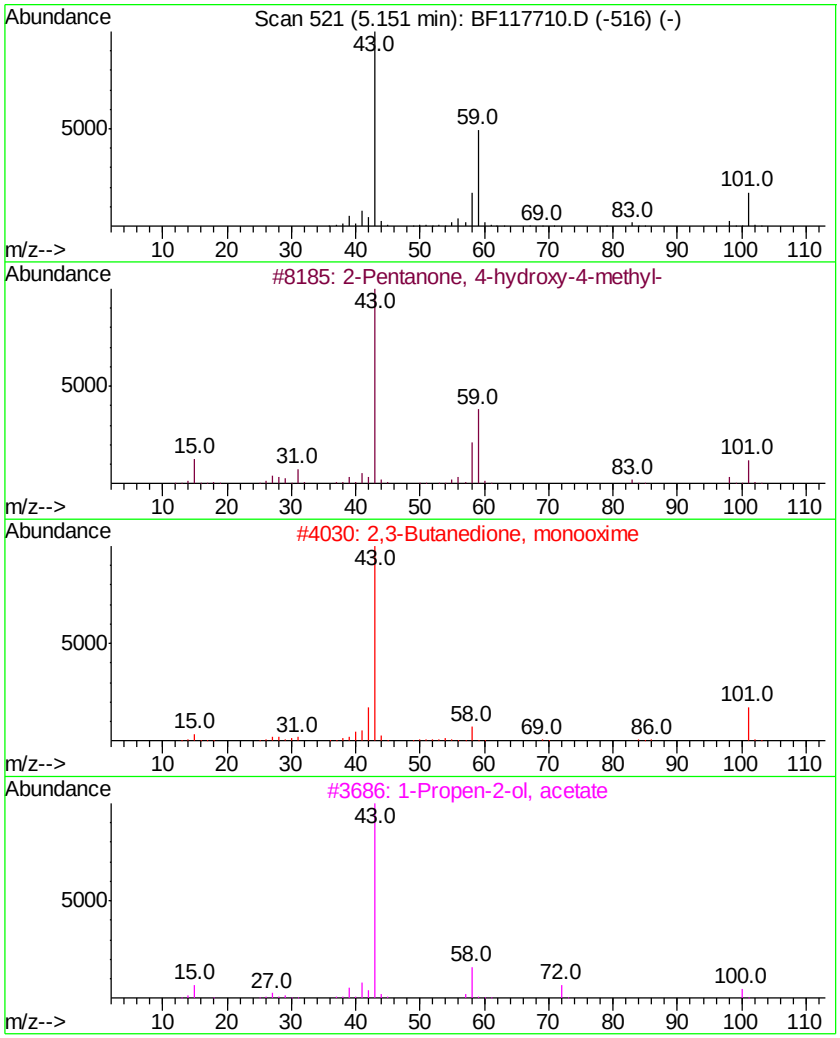
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

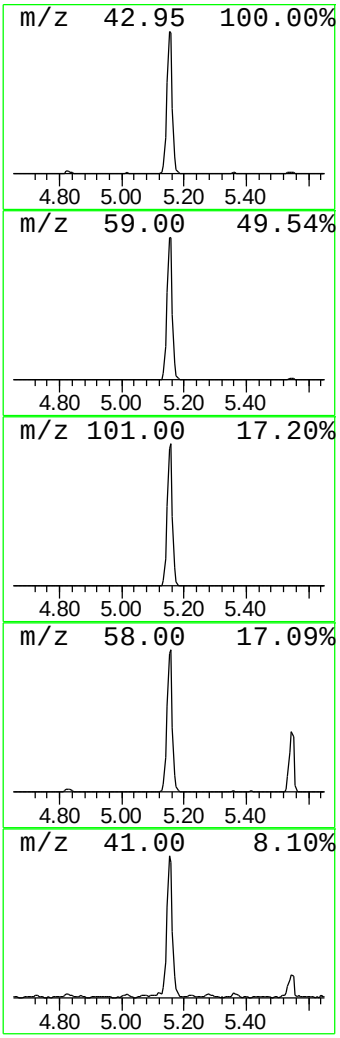
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	14.46 ng	1384350	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Allyl acetate	100	C5H8O2	000591-87-7	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	7





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
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Operator : JU
Sample : K5723-03
Misc :
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Instrument : BNA_F
ClientSampleId : 7-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
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TIC Library : C:\DATABASE\NIST11.L
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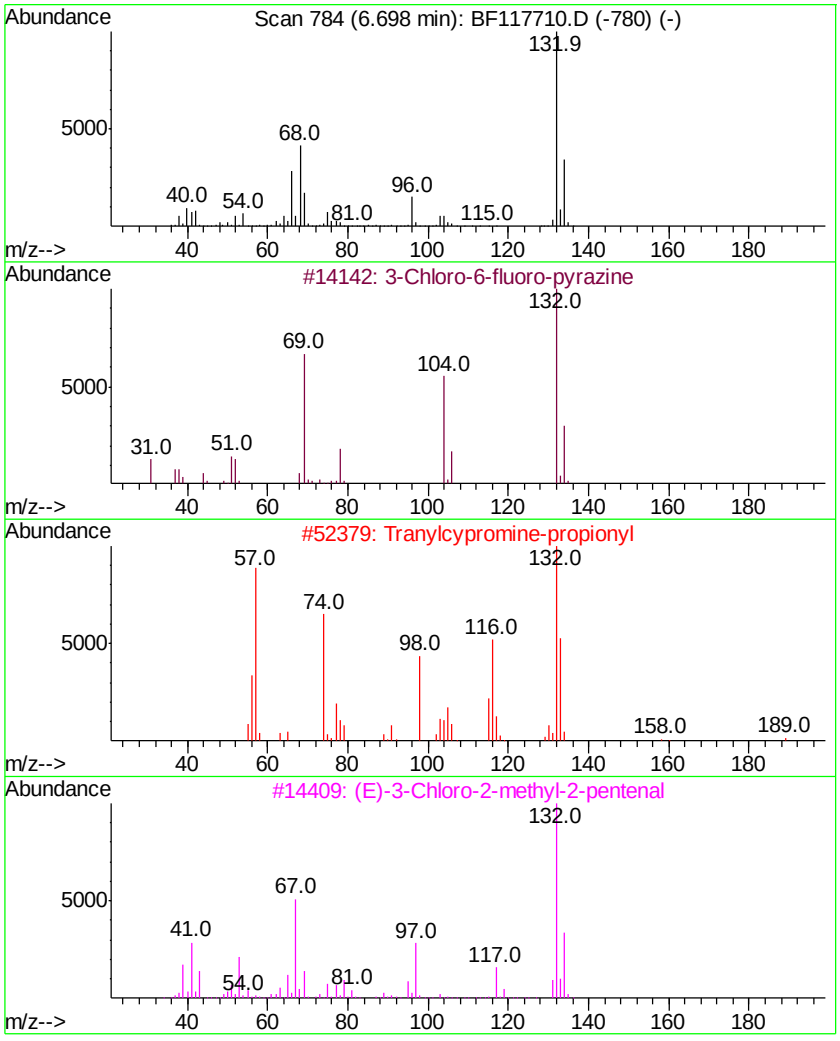
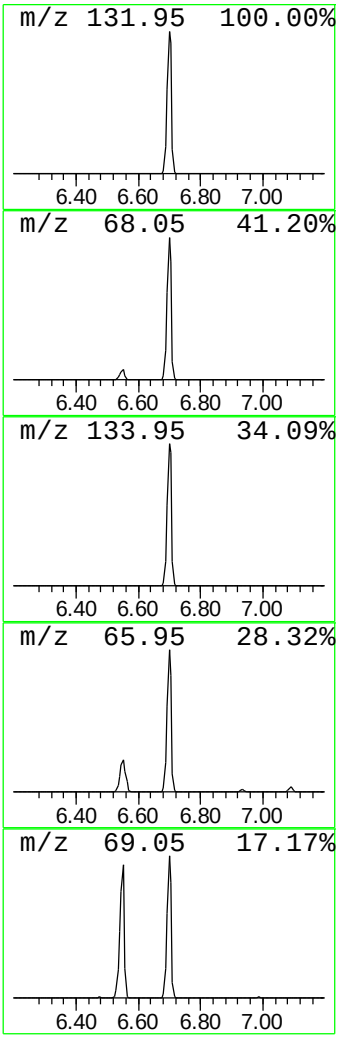
Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	67.85 ng	6494370	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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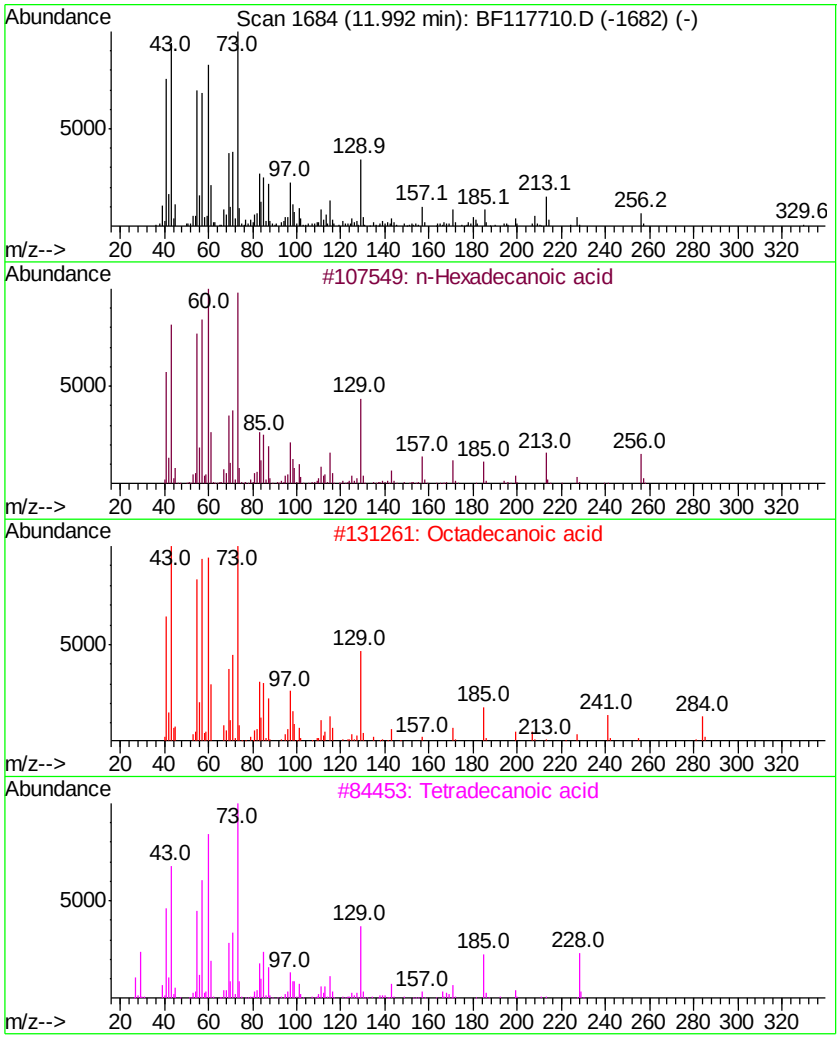
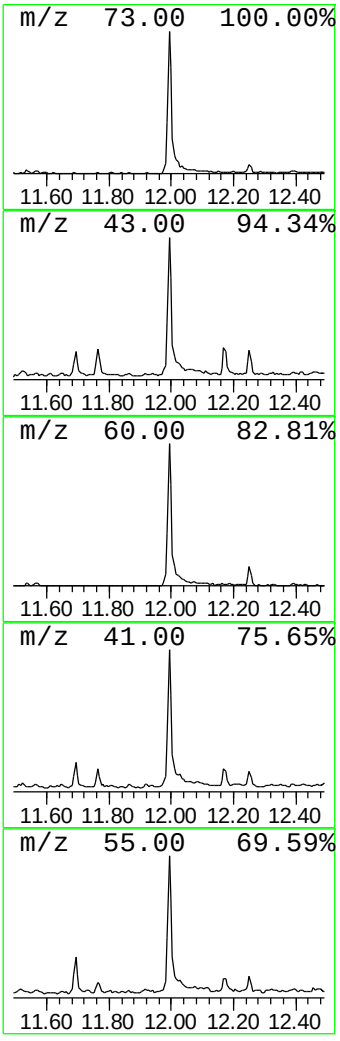
Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	3.66 ng	535595	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





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TIC Library : C:\DATABASE\NIST11.L
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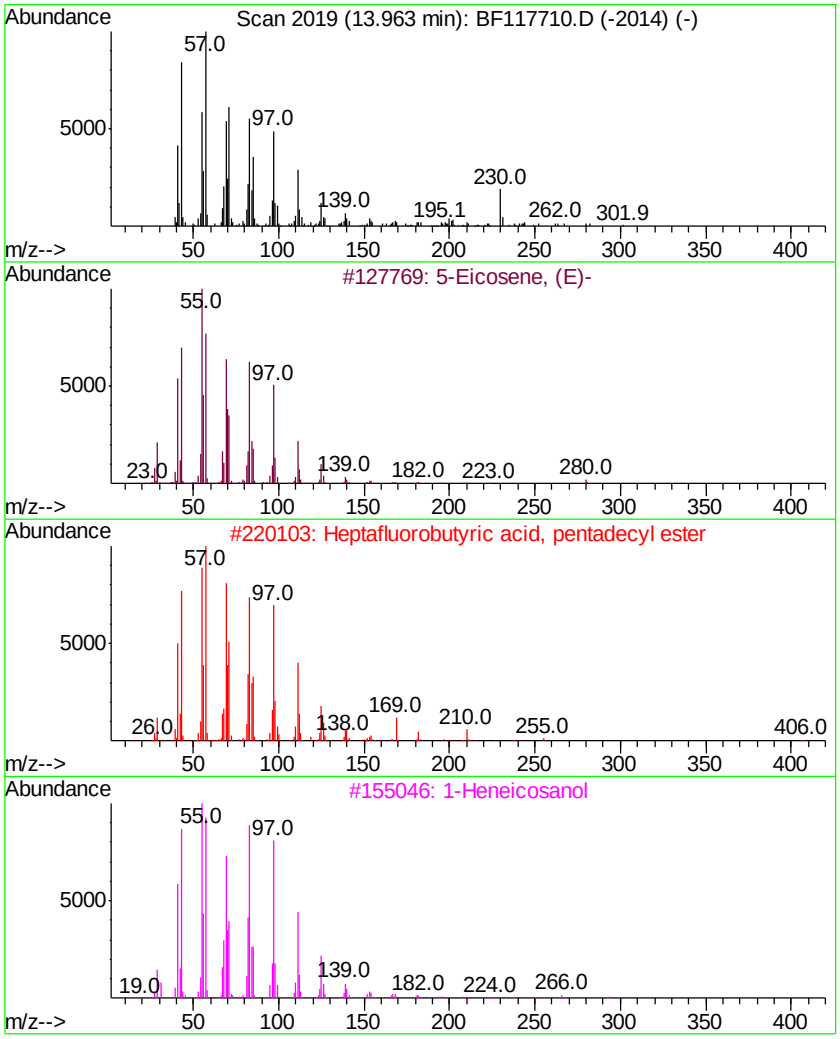
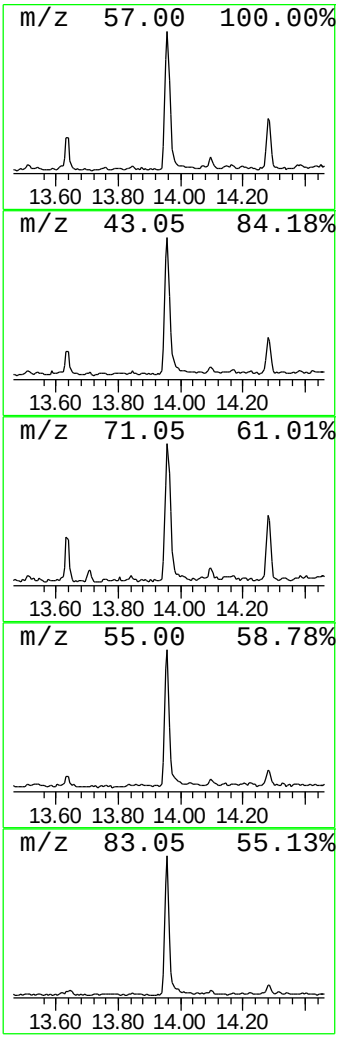
****

Peak Number 6 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	4.88 ng	577515	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91





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

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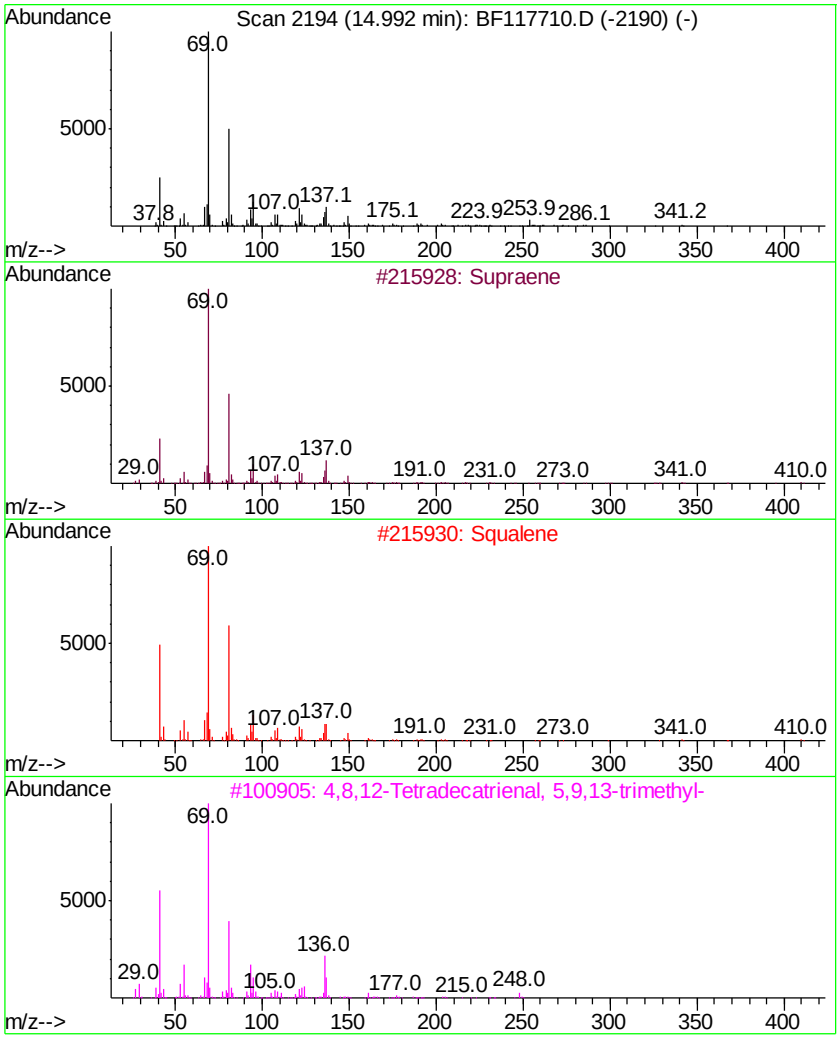
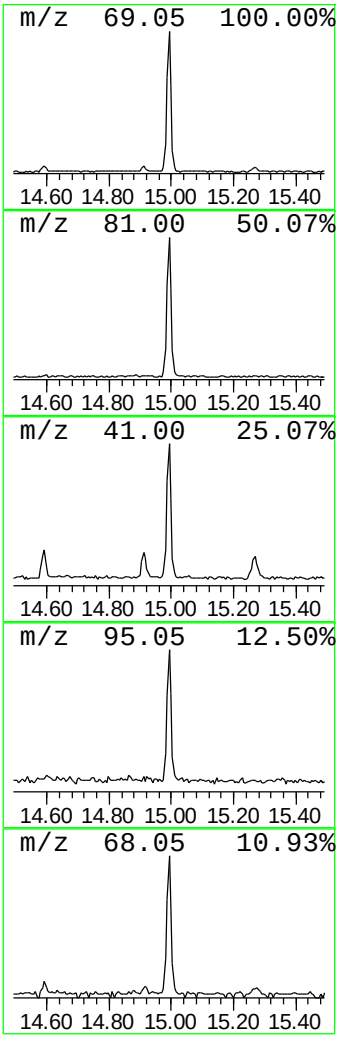
Peak Number 7 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	3.98 ng	464065	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	53





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.25	20.5	ng	1964820	1	6.93	1914320	20.0
2-Pentanone, 4-hy...	5.15	14.5	ng	1384350	1	6.93	1914320	20.0
unknown6.70	6.70	67.8	ng	6494370	1	6.93	1914320	20.0
n-Hexadecanoic acid	11.99	3.7	ng	535595	4	11.47	2928000	20.0
5-Eicosene, (E)-	13.96	4.9	ng	577515	5	14.12	2368300	20.0
Supraene	14.99	4.0	ng	464065	6	15.63	2331950	20.0