LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117713.D
Acq On : 7 Nov 2019 19:07
Operator : JU
Sample : K5723-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-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	2.222	18	23	39	rVB	1084510	1483638	28.60%	2.648%
2	5.145	515	520	528	rVB	907309	996491	19.21%	1.778%
3	5.545	583	588	591	rBV	4489469	4519026	87.11%	8.064%
4	6.545	753	758	763	rBV	4955566	4901026	94.47%	8.746%
5	6.698	780	784	787	rBV	5536236	4856868	93.62%	8.667%
6	6.934	820	824	827	rVB	2236394	1677761	32.34%	2.994%
7	7.092	847	851	854	rVB	4315506	3780542	72.87%	6.746%
8	7.492	914	919	922	rBV	3521806	2902379	55.95%	5.179%
9	8.222	1039	1043	1046	rBV	2581237	2206446	42.53%	3.937%
10	9.298	1222	1226	1229	rVB	6270260	5187726	100.00%	9.258%
11	9.686	1289	1292	1295	rBV	736284	533352	10.28%	0.952%
12	9.980	1338	1342	1345	rBV	3069507	2520234	48.58%	4.497%
13	10.769	1472	1476	1479	rBV	3902586	3338228	64.35%	5.957%
14	10.869	1489	1493	1495	rBV	116776	100127	1.93%	0.179%
15	11.469	1591	1595	1598	rBV	2994454	2592608	49.98%	4.627%
16	11.492	1598	1599	1602	rVV	261176	169208	3.26%	0.302%
17	11.539	1602	1607	1610	rVB3	123989	130702	2.52%	0.233%
18	11.692	1629	1633	1636	rBV	68609	66951	1.29%	0.119%
19	11.974	1678	1681	1682	rBV	75094	75765	1.46%	0.135%
20	11.992	1682	1684	1689	rVB2	351873	329082	6.34%	0.587%
21	12.080	1696	1699	1702	rBV2	77287	86447	1.67%	0.154%
22	12.604	1786	1788	1795	rVB2	52139	64446	1.24%	0.115%
23	12.686	1799	1802	1807	rVV	545699	456278	8.80%	0.814%
24	12.780	1815	1818	1821	rBV2	95700	93503	1.80%	0.167%
25	12.916	1836	1841	1844	rBV	531828	483331	9.32%	0.863%
26	13.063	1861	1866	1869	rBV	5364891	4869318	93.86%	8.689%
27	13.133	1874	1878	1882	rBV3	58017	86950	1.68%	0.155%
28	13.751	1980	1983	1988	rVB	78556	78675	1.52%	0.140%
29	13.868	1998	2003	2005	rBV2	43507	72782	1.40%	0.130%
30	13.957	2014	2018	2026	rBV	518330	522201	10.07%	0.932%
31	14.115	2040	2045	2048	rBV	2273317	2313075	44.59%	4.128%
32	14.139	2048	2049	2058	rVB	248601	230146	4.44%	0.411%
33	14.280	2071	2073	2080	rVB3	84400	97211	1.87%	0.173%
34	14.539	2114	2117	2121	rVB2	75655	74288	1.43%	0.133%

LSC Area Percent Report

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Instrument : BNA_F
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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

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Peak separation: 5

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

35	14.592	2123	2126	2130	rVB	125058	131259	2.53%	0.234%
36	14.910	2177	2180	2190	rVB3	104048	142506	2.75%	0.254%
37	14.992	2190	2194	2199	rBV	248078	266957	5.15%	0.476%
38	15.174	2221	2225	2229	rBV	223268	353456	6.81%	0.631%
39	15.268	2237	2241	2243	rBV2	87025	109702	2.11%	0.196%
40	15.492	2276	2279	2286	rVB	149972	175088	3.38%	0.312%
41	15.557	2286	2290	2296	rVB	134931	175795	3.39%	0.314%
42	15.627	2296	2302	2306	rBV	1698666	2184395	42.11%	3.898%
43	15.668	2306	2309	2319	rVB3	101338	169662	3.27%	0.303%
44	16.133	2383	2388	2392	rBV2	71417	118067	2.28%	0.211%
45	16.174	2392	2395	2400	rVV5	38803	64849	1.25%	0.116%
46	17.145	2555	2560	2569	rVB2	69898	157530	3.04%	0.281%
47	17.603	2635	2638	2646	rVB	53351	91806	1.77%	0.164%

Sum of corrected areas: 56037883

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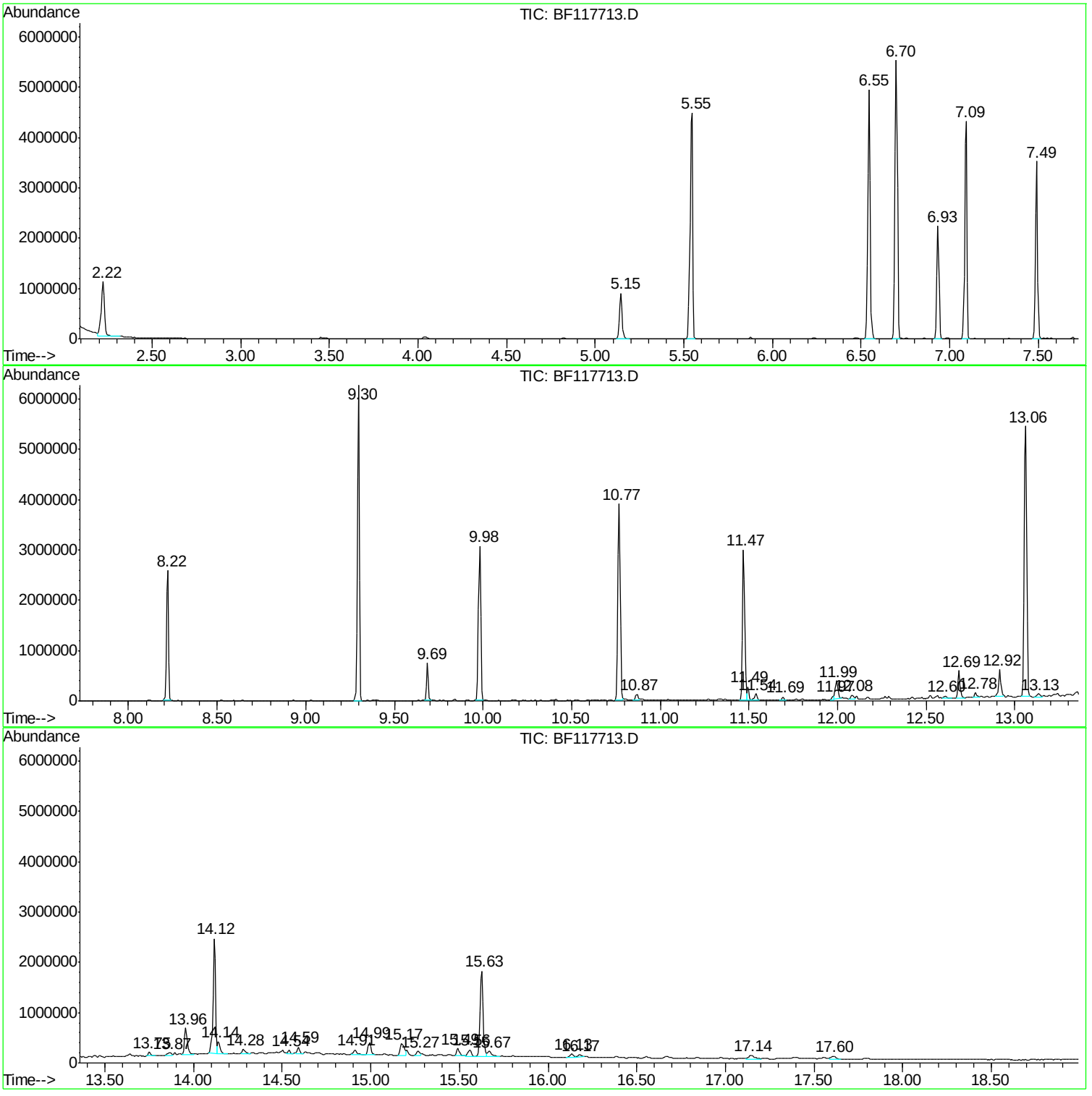
ClientSampleId : 8-C

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



Library Search Compound Report

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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-C

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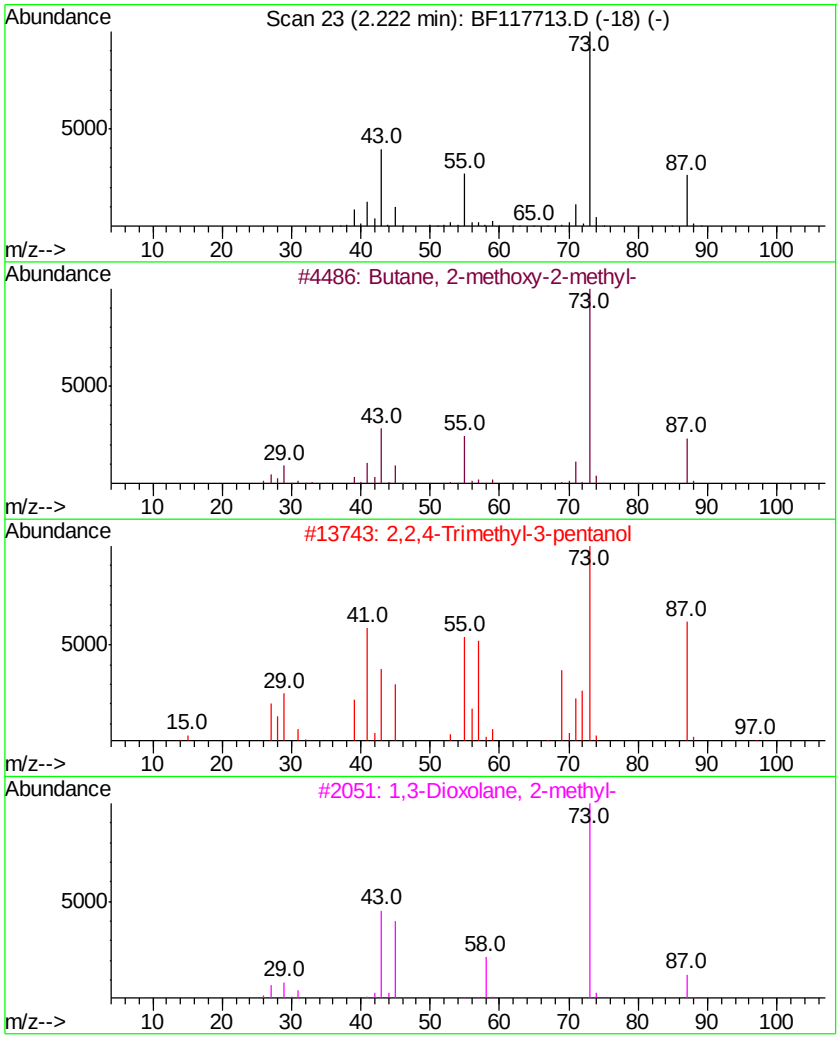
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

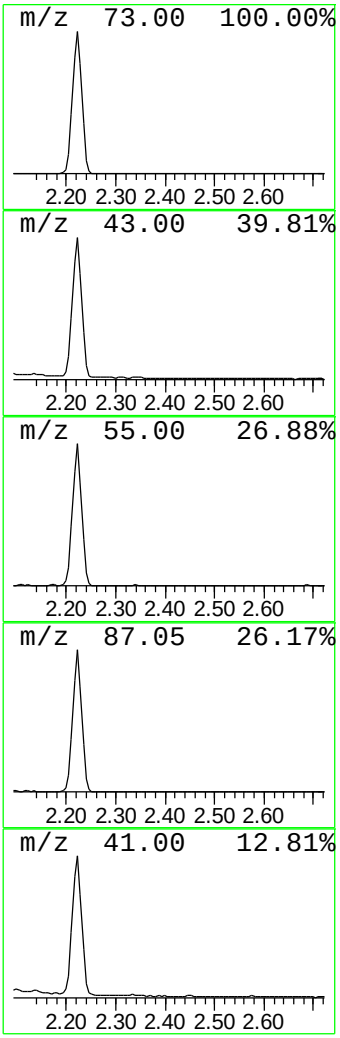
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	17.69 ng	1483640	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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-C

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

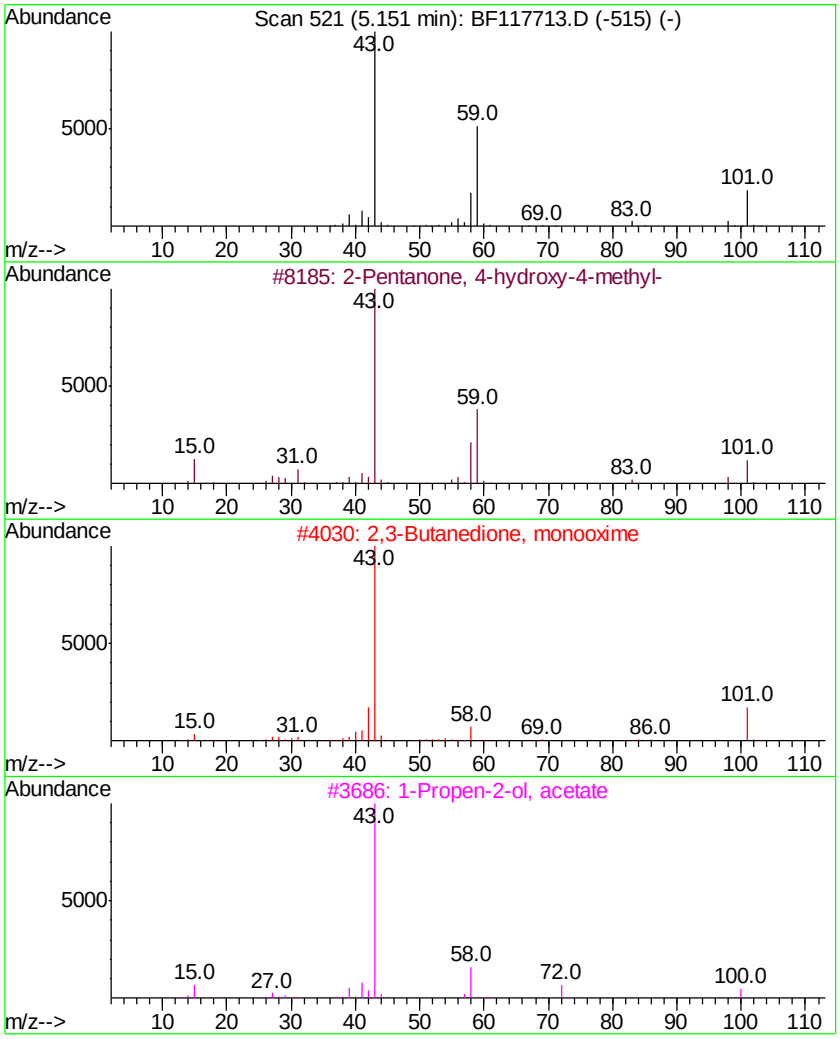
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

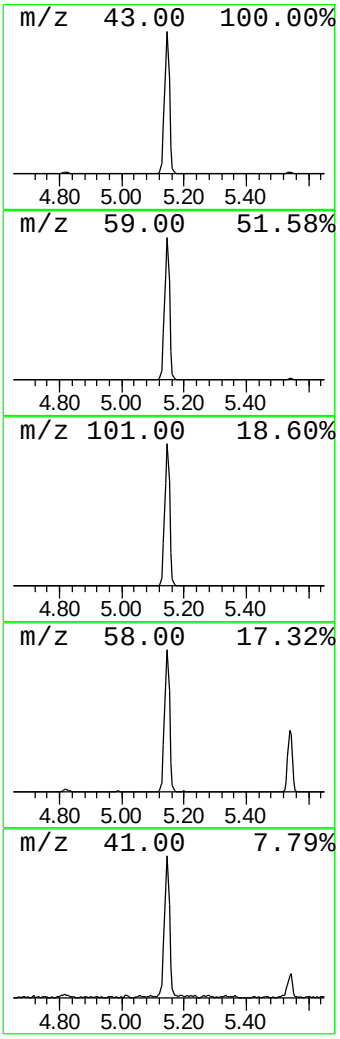
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	11.88 ng	996491	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	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	Allyl acetate	100	C5H8O2	000591-87-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
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Operator : JU
Sample : K5723-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-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
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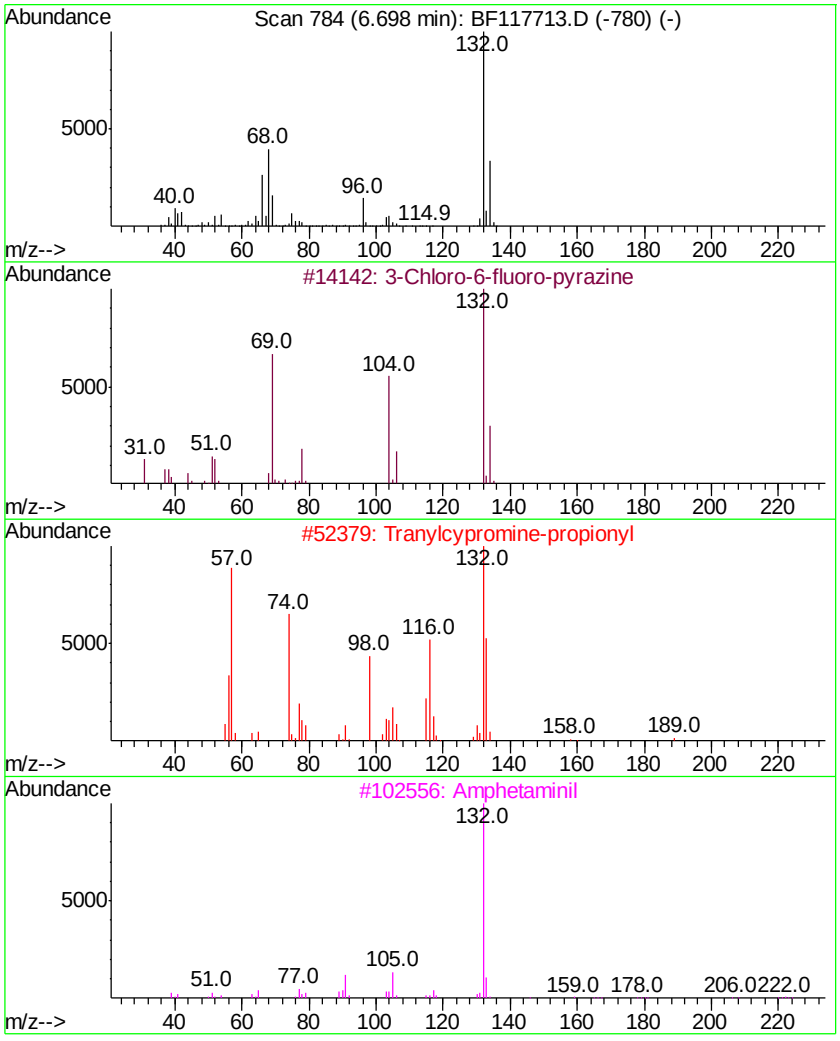
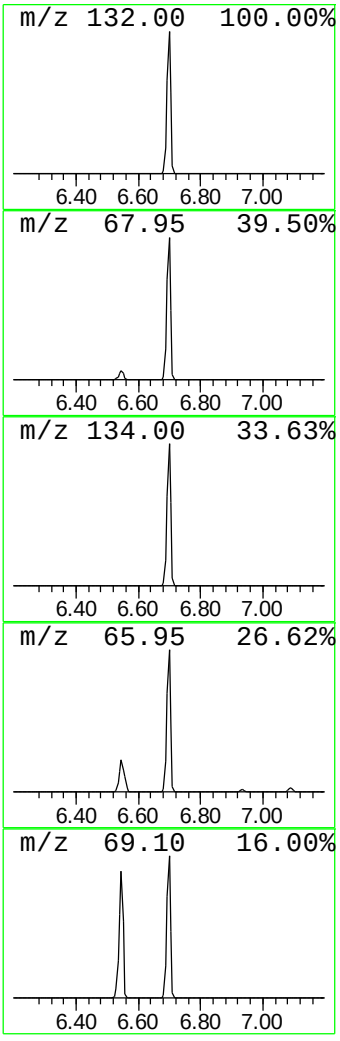
****

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	57.90 ng	4856870	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	Amphetaminil	250	C17H18N2	017590-01-1	12
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





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TIC Library : C:\DATABASE\NIST11.L
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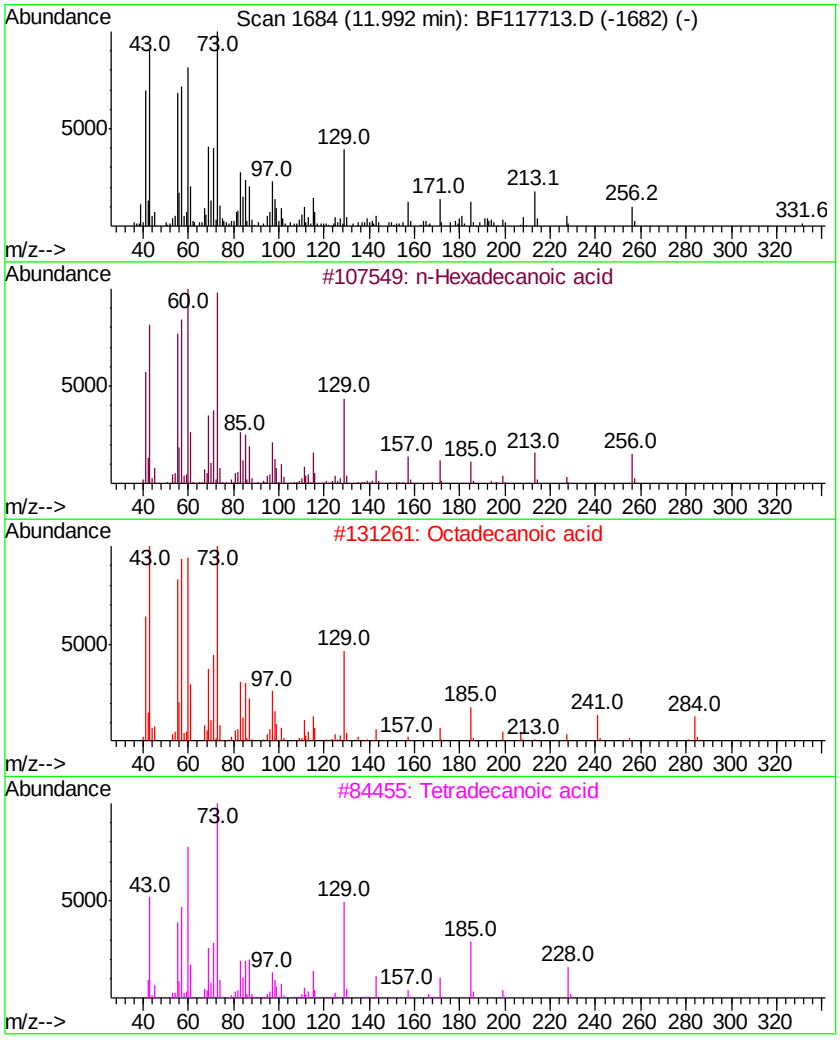
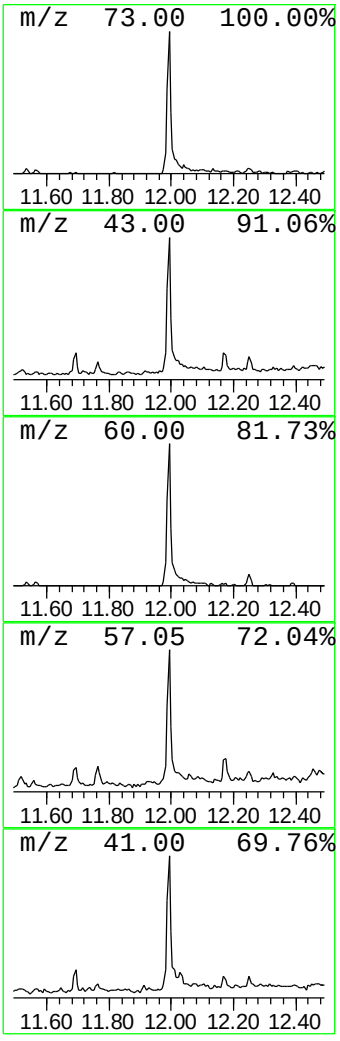
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.54 ng	329082	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Tridecanoic acid	214	C13H26O2	000638-53-9	91





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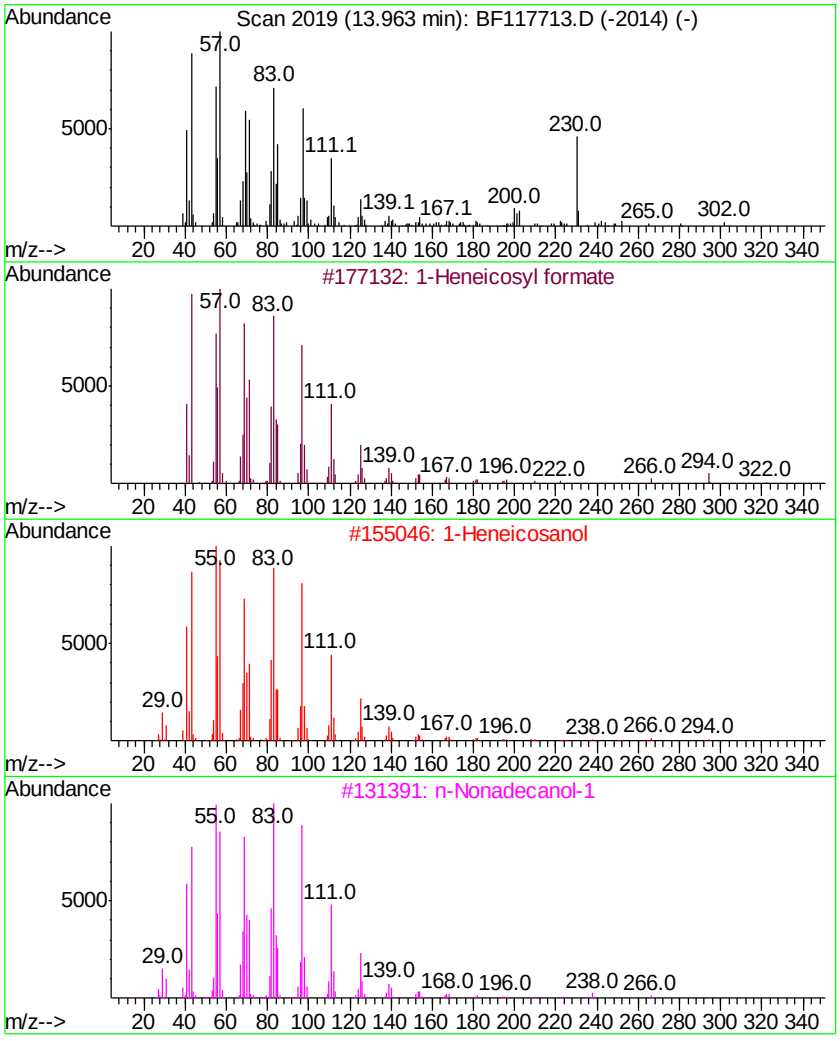
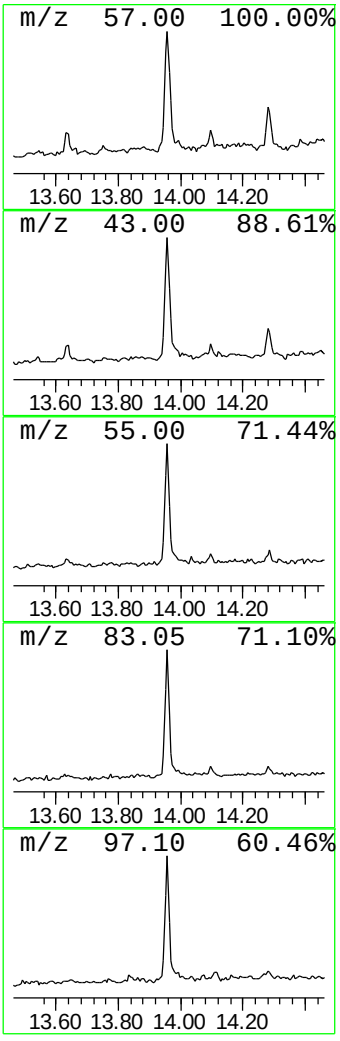
****

Peak Number 6 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	4.52 ng	522201	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	93





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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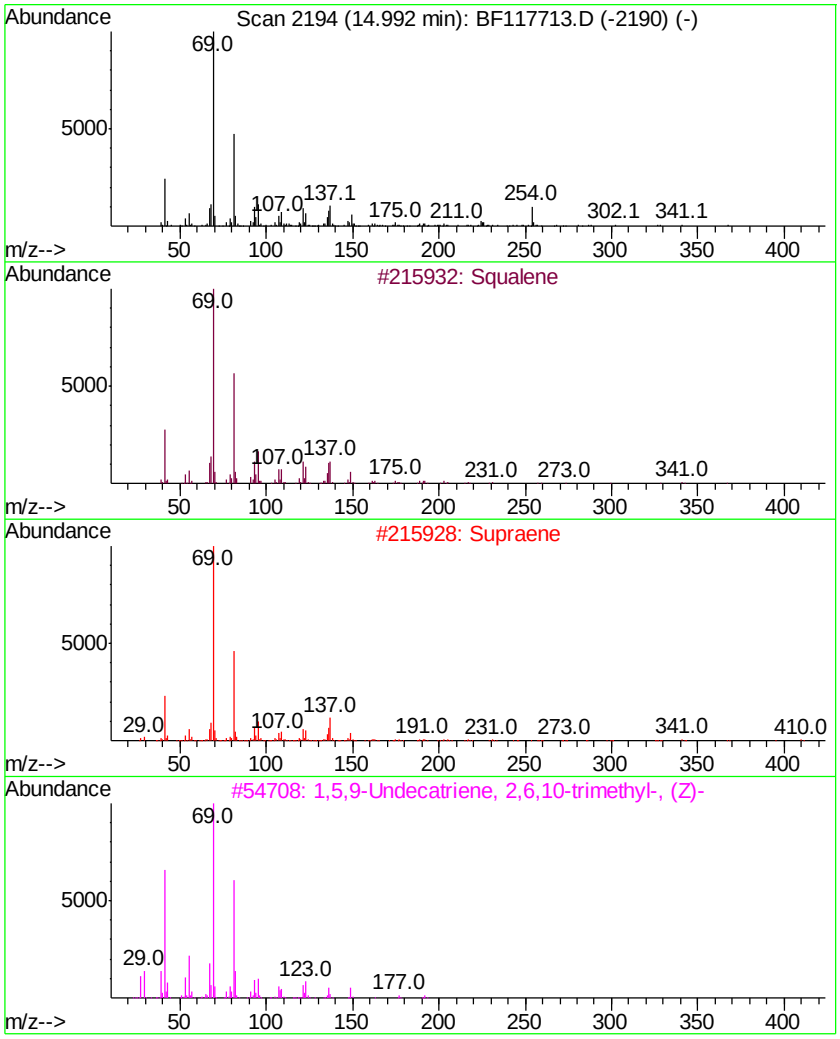
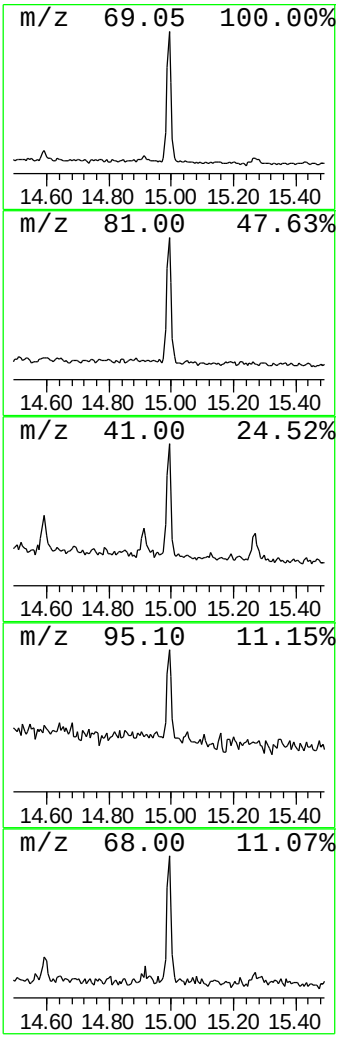
Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	2.44 ng	266957	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	93
2	Supraene	410	C30H50	007683-64-9	90
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	81
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
5	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72





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...	2.22	17.7	ng	1483640	1	6.93	1677760	20.0
2-Pentanone, 4-hy...	5.15	11.9	ng	996491	1	6.93	1677760	20.0
unknown6.70	6.70	57.9	ng	4856870	1	6.93	1677760	20.0
n-Hexadecanoic acid	11.99	2.5	ng	329082	4	11.47	2592610	20.0
1-Heneicosyl formate	13.96	4.5	ng	522201	5	14.12	2313080	20.0
Squalene	14.99	2.4	ng	266957	6	15.63	2184400	20.0