LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

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-BF101819.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	5.357	553	556	586	rBV	303756	586536	84.43%	5.505%
2	6.386	728	731	748	rBV	418074	694114	99.91%	6.515%
3	6.504	748	751	760	rVB	683591	694725	100.00%	6.520%
4	6.728	785	789	800	rBV	188869	186320	26.82%	1.749%
5	6.881	811	815	831	rBV	556669	576061	82.92%	5.407%
6	7.298	883	886	906	rBV	248876	400384	57.63%	3.758%
7	8.010	1004	1007	1024	rBV	160139	238661	34.35%	2.240%
8	9.080	1186	1189	1209	rBV	581968	627135	90.27%	5.886%
9	9.410	1242	1245	1248	rBV	58447	46308	6.67%	0.435%
10	9.486	1252	1258	1267	rBV	55565	68630	9.88%	0.644%
11	9.763	1301	1305	1318	rBV	279263	296068	42.62%	2.779%
12	9.874	1322	1324	1327	rVB	15110	11037	1.59%	0.104%
13	10.480	1423	1427	1430	rBV2	8954	10516	1.51%	0.099%
14	10.557	1437	1440	1456	rBV	294691	384809	55.39%	3.612%
15	10.669	1456	1459	1462	rVV	21670	19186	2.76%	0.180%
16	10.786	1475	1479	1481	rBV	9120	7369	1.06%	0.069%
17	11.039	1520	1522	1526	rVB	8532	7373	1.06%	0.069%
18	11.227	1545	1554	1555	rBV3	6523	11519	1.66%	0.108%
19	11.251	1555	1558	1565	rBV	238266	259072	37.29%	2.432%
20	11.363	1573	1577	1589	rVB4	25312	48572	6.99%	0.456%
21	11.686	1628	1632	1641	rBV6	29940	72359	10.42%	0.679%
22	11.757	1641	1644	1645	rVV	19329	18229	2.62%	0.171%
23	11.780	1645	1648	1656	rVB	81648	94395	13.59%	0.886%
24	11.880	1662	1665	1669	rVB2	15296	13837	1.99%	0.130%
25	11.945	1669	1676	1680	rVV5	3612	7166	1.03%	0.067%
26	11.980	1680	1682	1686	rVB2	12566	11209	1.61%	0.105%
27	12.092	1698	1701	1707	rBV	73724	65034	9.36%	0.610%
28	12.180	1714	1716	1719	rVB2	12443	9383	1.35%	0.088%
29	12.298	1733	1736	1737	rBV2	7252	7361	1.06%	0.069%
30	12.327	1738	1741	1744	rVV2	35014	33860	4.87%	0.318%
31	12.374	1744	1749	1752	rVB2	10107	12154	1.75%	0.114%
32	12.492	1763	1769	1770	rBV3	18286	21546	3.10%	0.202%
33	12.557	1777	1780	1781	rBV	19353	15360	2.21%	0.144%
34	12.574	1781	1783	1790	rVB	22968	21944	3.16%	0.206%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

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-BF101819.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.704	1802	1805	1809	rVB2	6934	8769	1.26%	0.082%
36	12.827	1823	1826	1835	rVB	501971	468565	67.45%	4.398%
37	13.051	1858	1864	1870	rBV2	44868	79102	11.39%	0.742%
38	13.151	1878	1881	1887	rVB4	13927	17633	2.54%	0.165%
39	13.257	1892	1899	1902	rBV	208379	223582	32.18%	2.098%
40	13.286	1902	1904	1913	rVB2	141291	177649	25.57%	1.667%
41	13.392	1918	1922	1926	rBV3	15669	20446	2.94%	0.192%
42	13.721	1975	1978	1990	rBV	270116	387401	55.76%	3.636%
43	13.898	2005	2008	2019	rBV	161512	191596	27.58%	1.798%
44	14.039	2027	2032	2034	rBV2	26411	31211	4.49%	0.293%
45	14.162	2050	2053	2056	rBV2	10641	8703	1.25%	0.082%
46	14.286	2072	2074	2080	rBV4	12219	15369	2.21%	0.144%
47	14.357	2080	2086	2099	rBV2	294376	532434	76.64%	4.997%
48	14.509	2110	2112	2116	rVB4	6346	7776	1.12%	0.073%
49	14.639	2129	2134	2137	rBV	77960	81923	11.79%	0.769%
50	14.674	2137	2140	2142	rVV4	17913	21179	3.05%	0.199%
51	14.709	2142	2146	2150	rVV	140983	138897	19.99%	1.304%
52	14.774	2154	2157	2161	rBV4	14068	13518	1.95%	0.127%
53	14.957	2183	2188	2191	rBV	247689	277654	39.97%	2.606%
54	14.992	2191	2194	2198	rVV2	101597	160434	23.09%	1.506%
55	15.033	2198	2201	2207	rVB	67038	78467	11.29%	0.736%
56	15.309	2242	2248	2250	rBV	93703	126553	18.22%	1.188%
57	15.339	2250	2253	2260	rVV	122280	186272	26.81%	1.748%
58	15.398	2261	2263	2269	rVB4	20245	27508	3.96%	0.258%
59	15.498	2276	2280	2283	rBV4	17499	22198	3.20%	0.208%
60	15.580	2288	2294	2297	rBV7	9267	15021	2.16%	0.141%
61	15.715	2310	2317	2322	rBV	178366	259214	37.31%	2.433%
62	15.780	2322	2328	2332	rVV2	69966	151668	21.83%	1.423%
63	15.827	2332	2336	2341	rVV	83081	131319	18.90%	1.232%
64	15.880	2341	2345	2351	rVV7	13468	29612	4.26%	0.278%
65	15.939	2353	2355	2358	rVB3	8279	7606	1.09%	0.071%
66	16.133	2386	2388	2390	rBV2	5974	7252	1.04%	0.068%
67	16.180	2390	2396	2400	rVV2	29260	54247	7.81%	0.509%
68	16.280	2409	2413	2414	rBV4	8253	10345	1.49%	0.097%
69	16.451	2437	2442	2449	rVB2	21226	34793	5.01%	0.327%
70	16.568	2456	2462	2473	rBV8	12537	33694	4.85%	0.316%
71	16.668	2474	2479	2484	rVV6	24275	47800	6.88%	0.449%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

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-BF101819.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	16.721	2484	2488	2495	rVB4	28316	57467	8.27%	0.539%
73	16.839	2502	2508	2509	rBV5	24136	35356	5.09%	0.332%
74	16.898	2513	2518	2523	rVV	58417	124011	17.85%	1.164%
75	16.956	2523	2528	2536	rVB3	78462	151506	21.81%	1.422%
76	17.280	2570	2583	2590	rBV4	102176	245452	35.33%	2.304%
77	17.362	2590	2597	2601	rBV10	11119	22163	3.19%	0.208%
78	17.527	2618	2625	2643	rBV10	63470	233702	33.64%	2.193%
79	17.886	2681	2686	2689	rBV5	10542	17986	2.59%	0.169%
80	18.050	2707	2714	2724	rVB8	16678	49288	7.09%	0.463%
81	18.386	2764	2771	2779	rVB6	18745	52172	7.51%	0.490%

Sum of corrected areas: 10654745

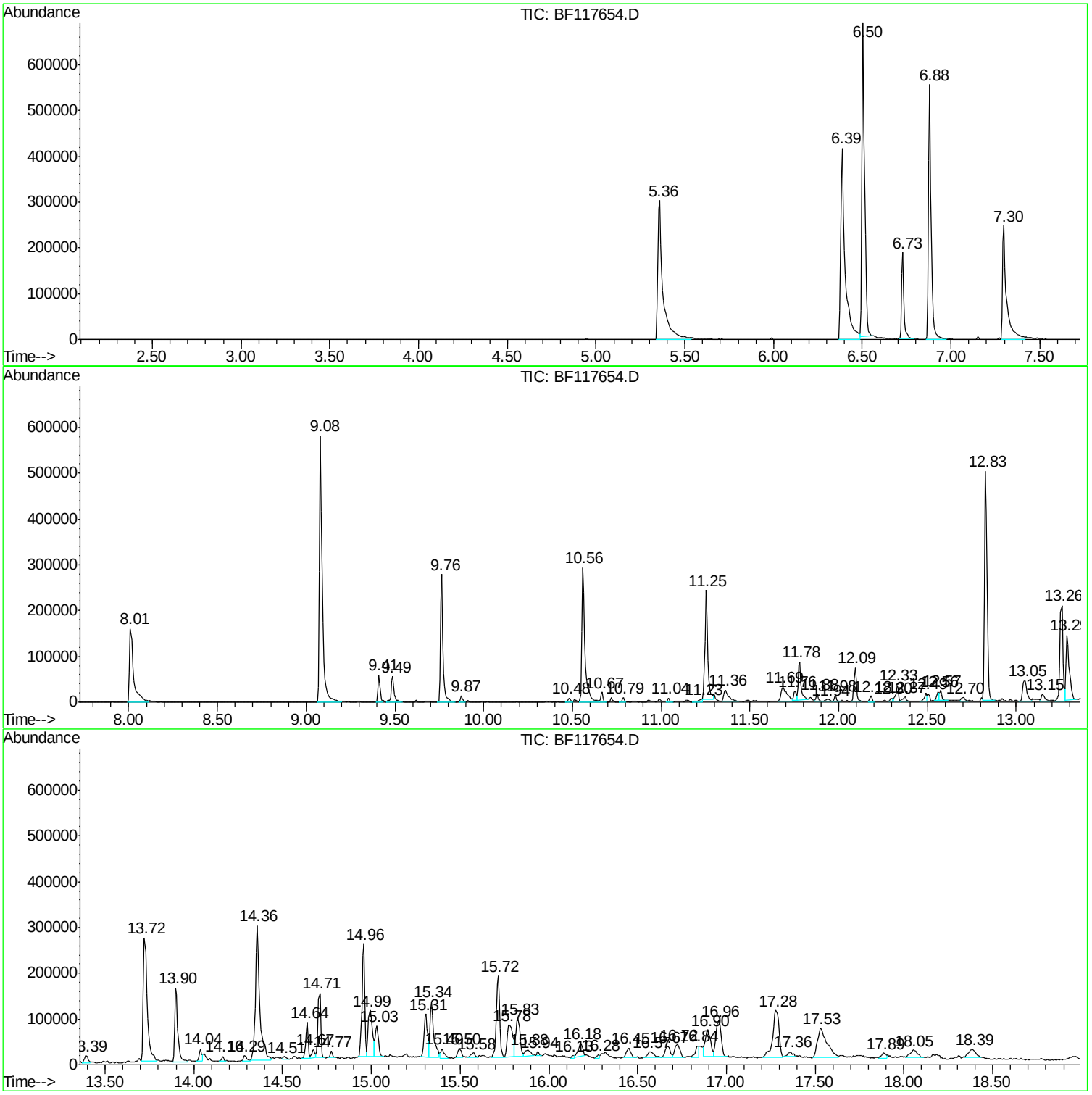
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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 F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

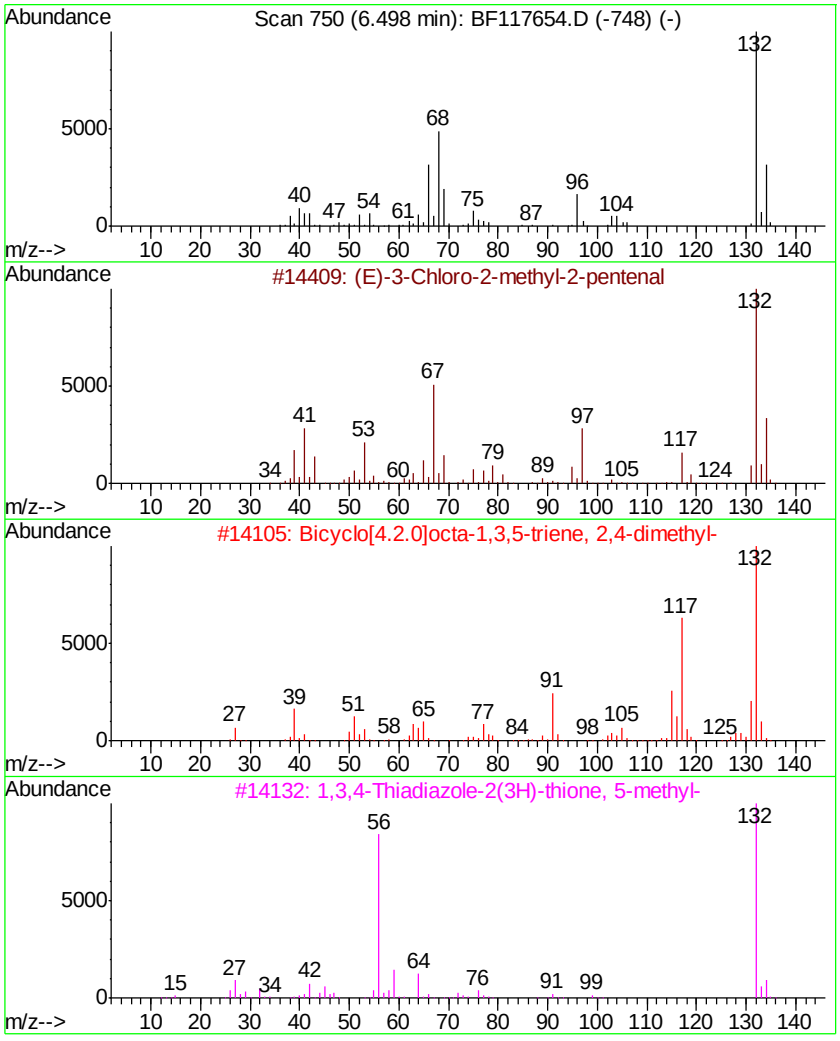
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

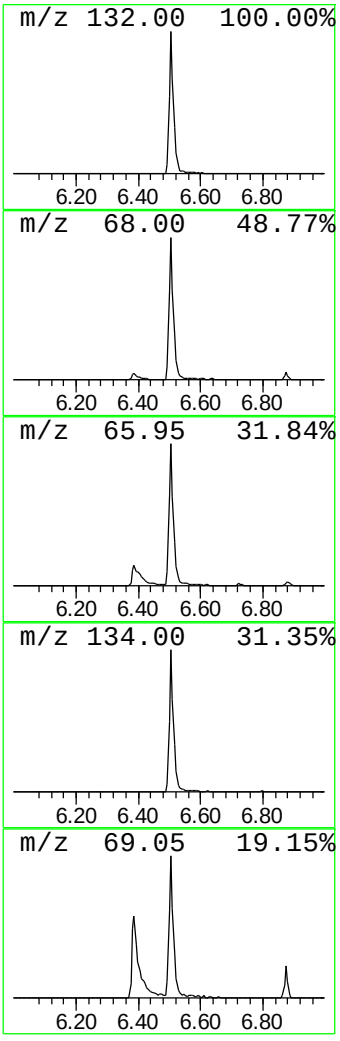
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	74.57 ng	694725	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

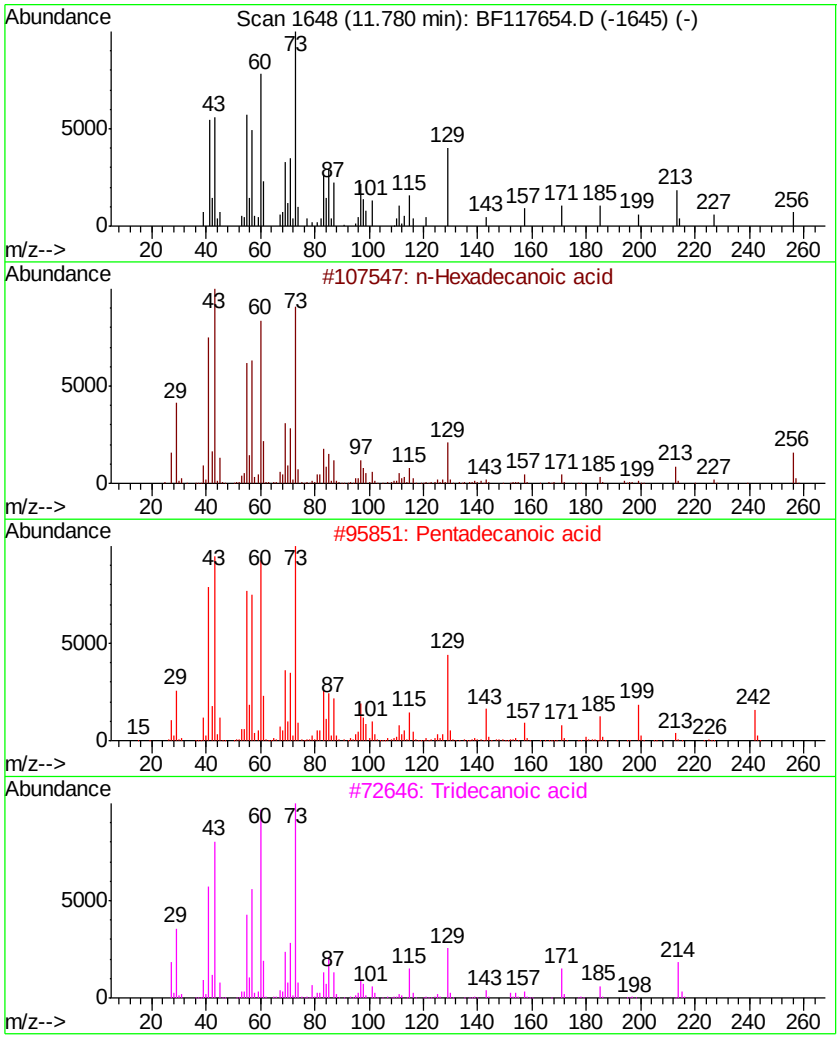
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

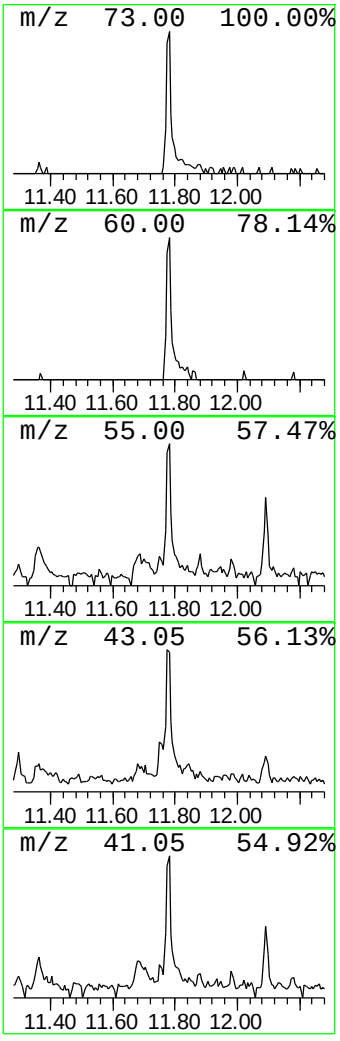
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	7.29 ng	94395	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

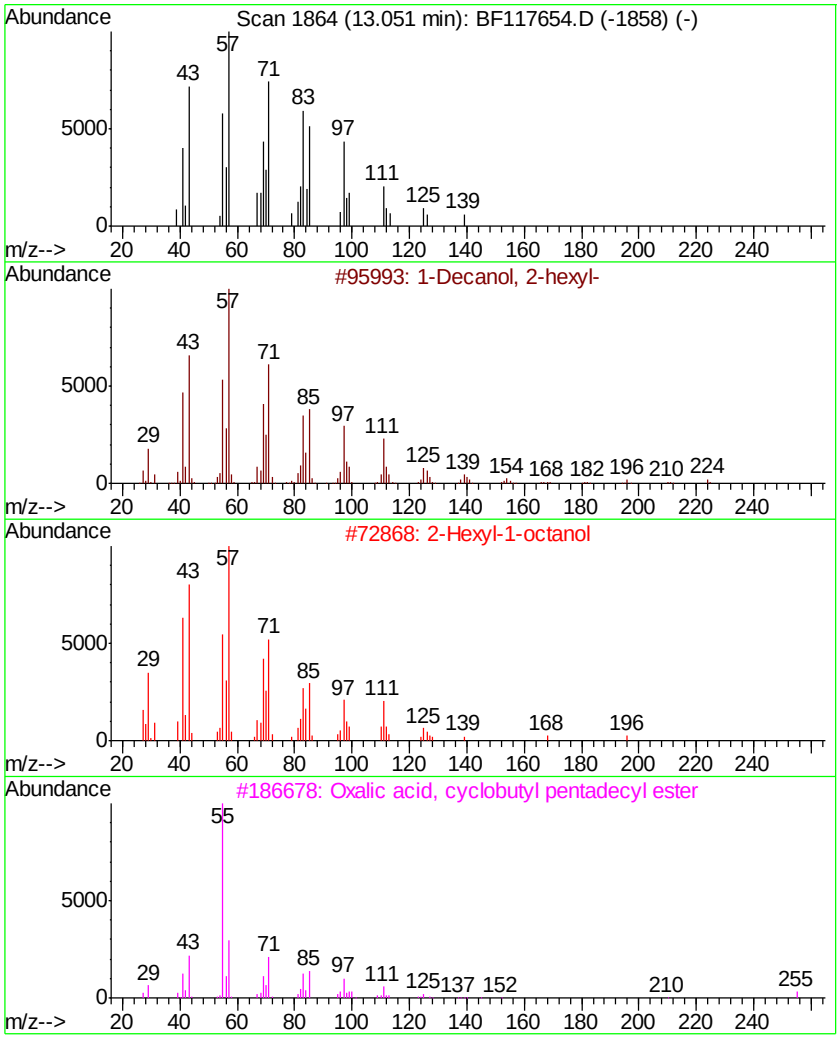
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

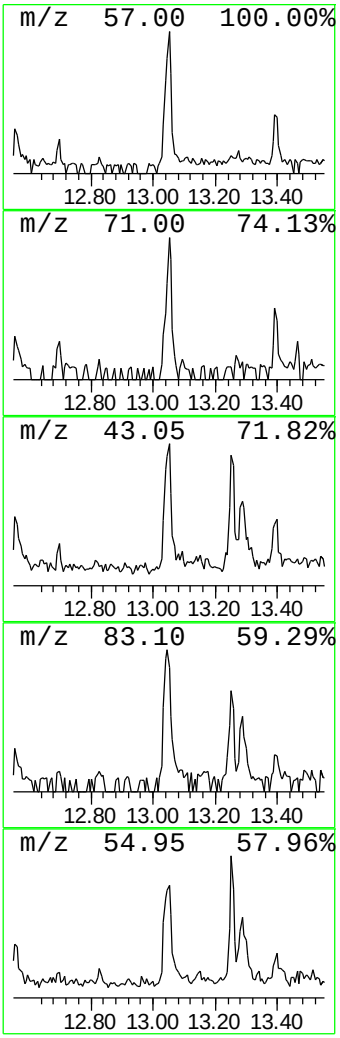
****

Peak Number 4 1-Decanol, 2-hexyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.05	8.26 ng	79102	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	68
2	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	64
3	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	64
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	58
5	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

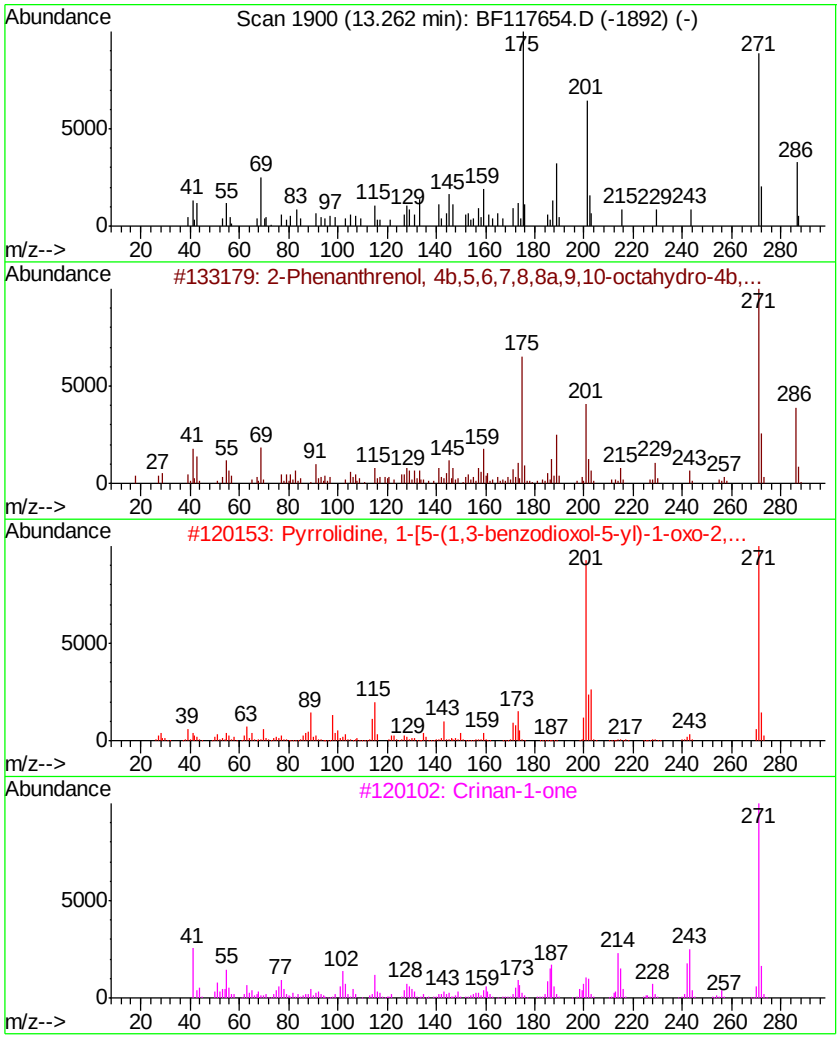
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

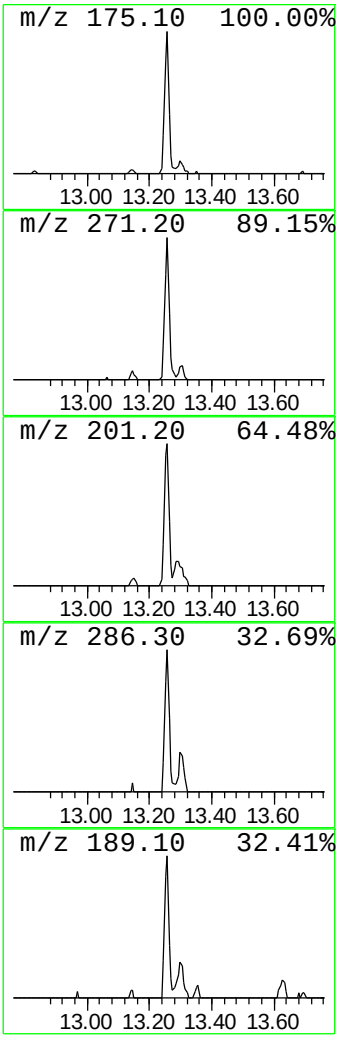
****

Peak Number 5 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	23.34 ng	223582	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	93
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	46
3	Crinan-1-one	271	C16H17NO3	098301-98-5	25
4	Dihydronormorphinone	271	C16H17NO3	014696-23-2	18
5	Desomorphine	271	C17H21NO2	000427-00-9	18





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

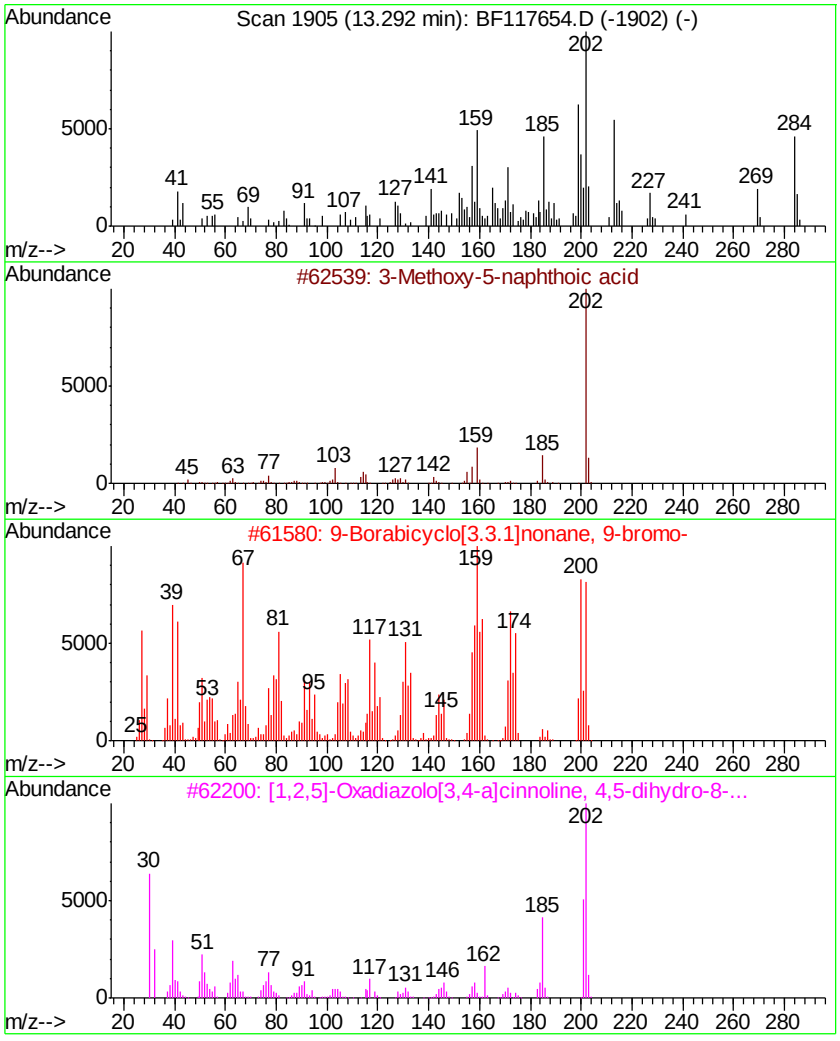
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

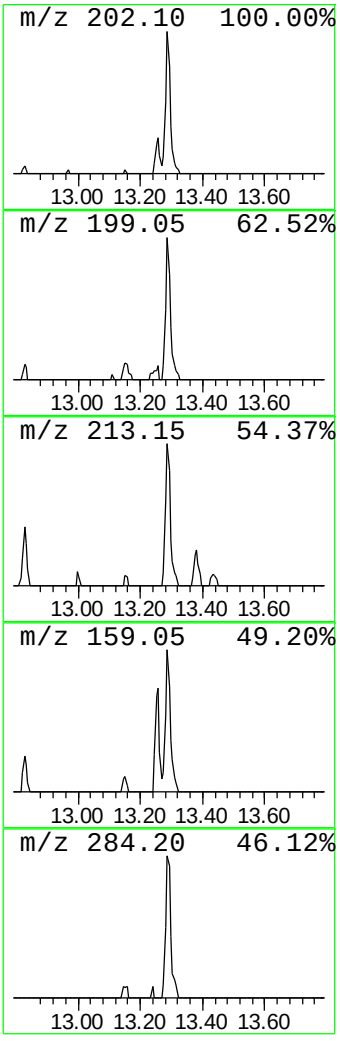
****

Peak Number 6 3-Methoxy-5-naphthoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	18.54 ng	177649	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methoxy-5-naphthoic acid	202	C12H10O3	007498-58-0	50
2	9-Borabicyclo[3.3.1]nonane, 9-br...	200	C8H14BBr	022086-45-9	35
3	[1,2,5]-Oxadiazolo[3,4-a]cinnoli...	202	C10H10N4O	1000260-59-4	27
4	1-Naphthalenecarboxylic acid, 2-...	202	C12H10O3	000947-62-6	27
5	1-Methyl-7,11-dithiaspiro[5,5] u...	202	C10H18S2	107678-22-8	20





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

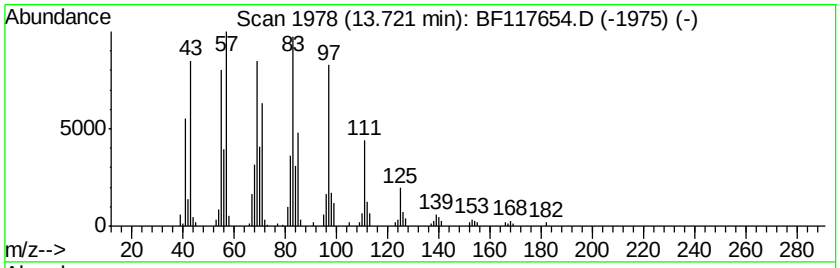
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

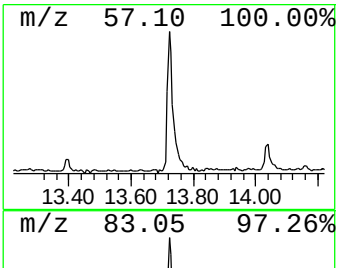
****

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	40.44 ng	387401	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
5	Behenic alcohol	326	C22H46O	000661-19-8	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

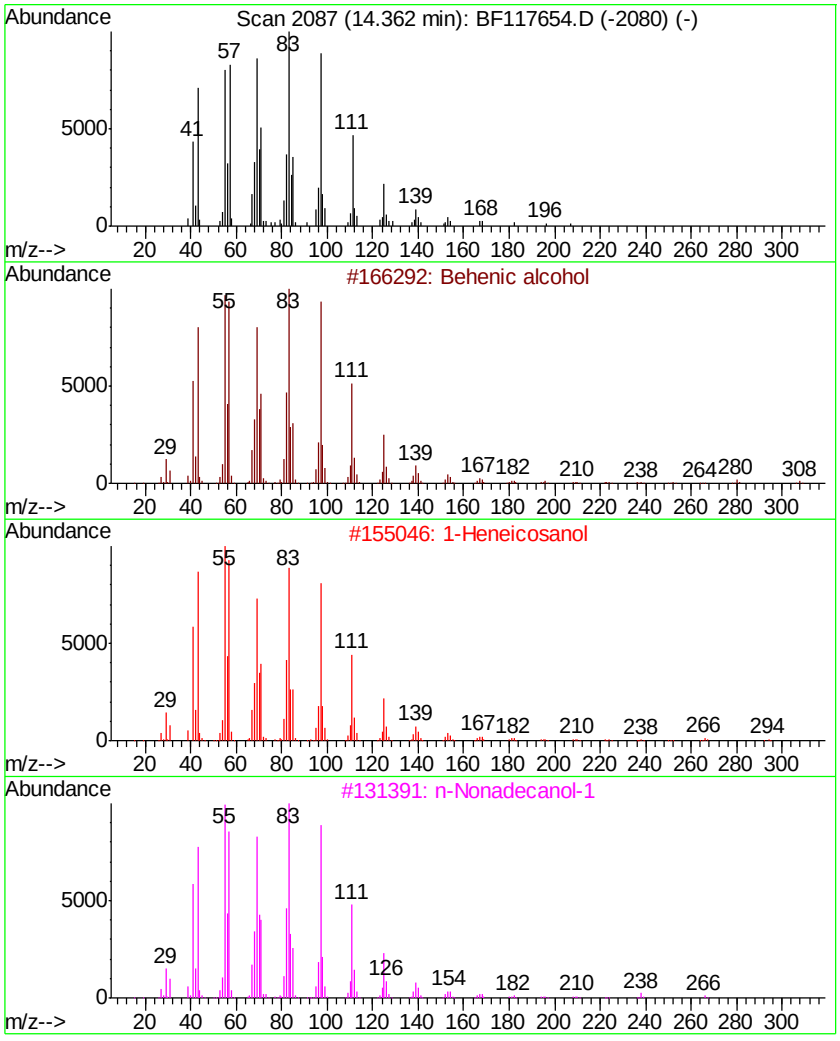
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

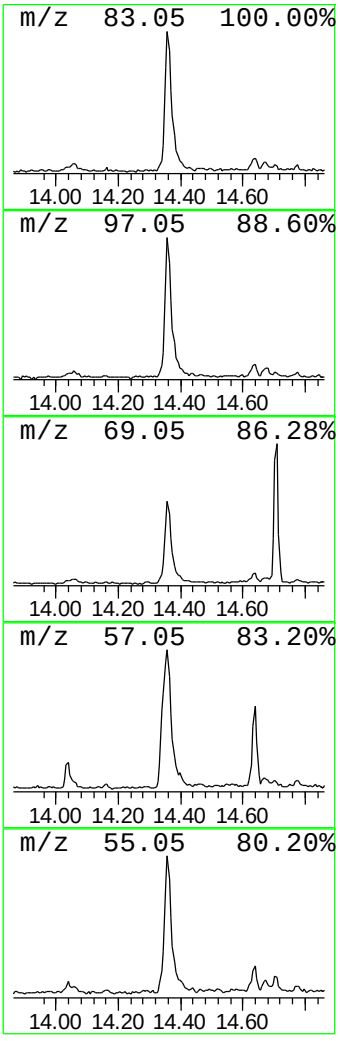
****

Peak Number 8 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	55.58 ng	532434	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

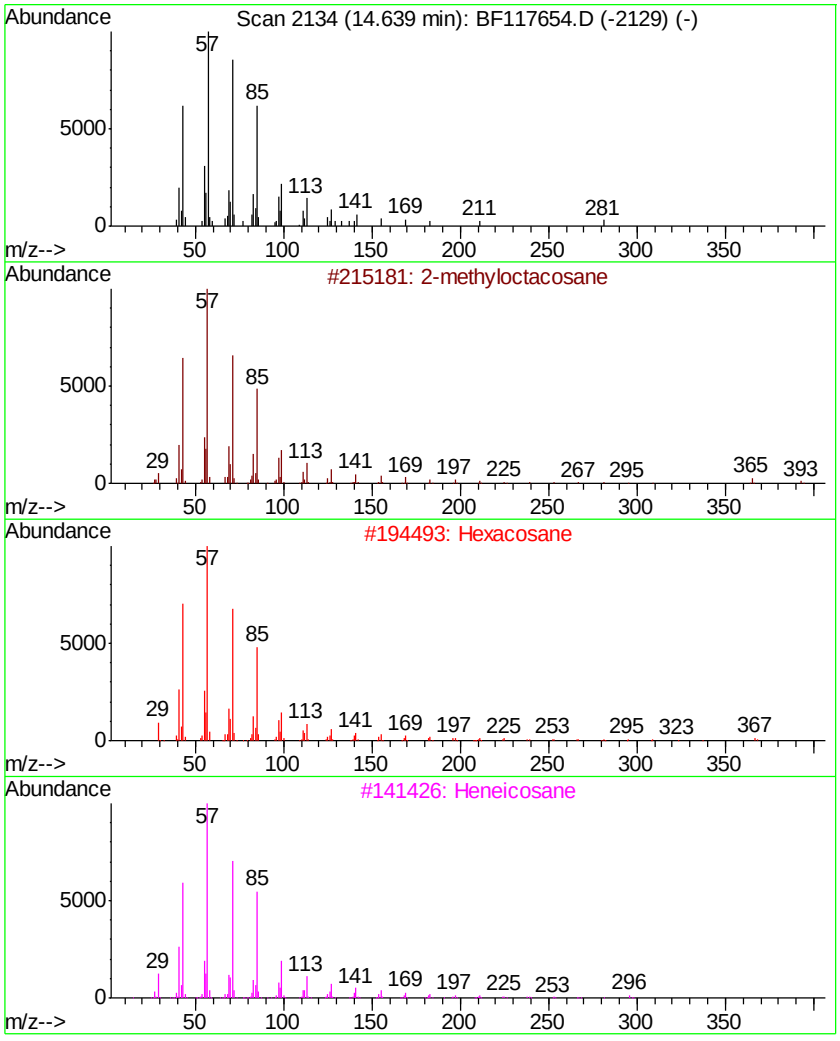
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

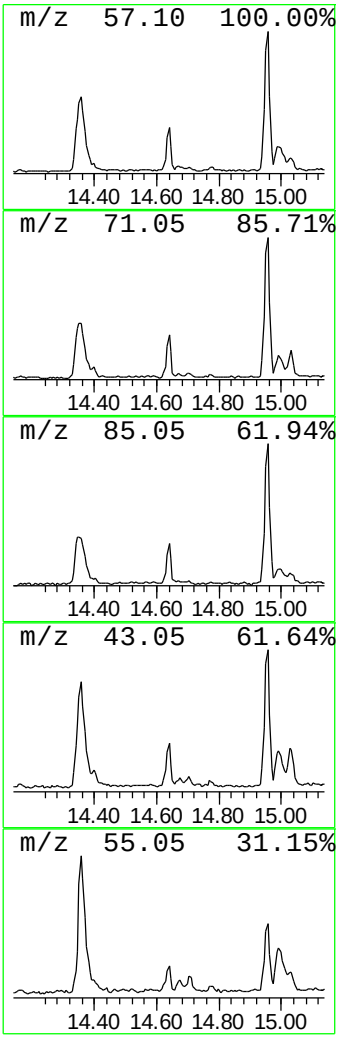
****

Peak Number 9 2-methyloctacosane Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	8.80 ng	81923	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptacosane	380	C27H56	000593-49-7	90
5	Heptadecane	240	C17H36	000629-78-7	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

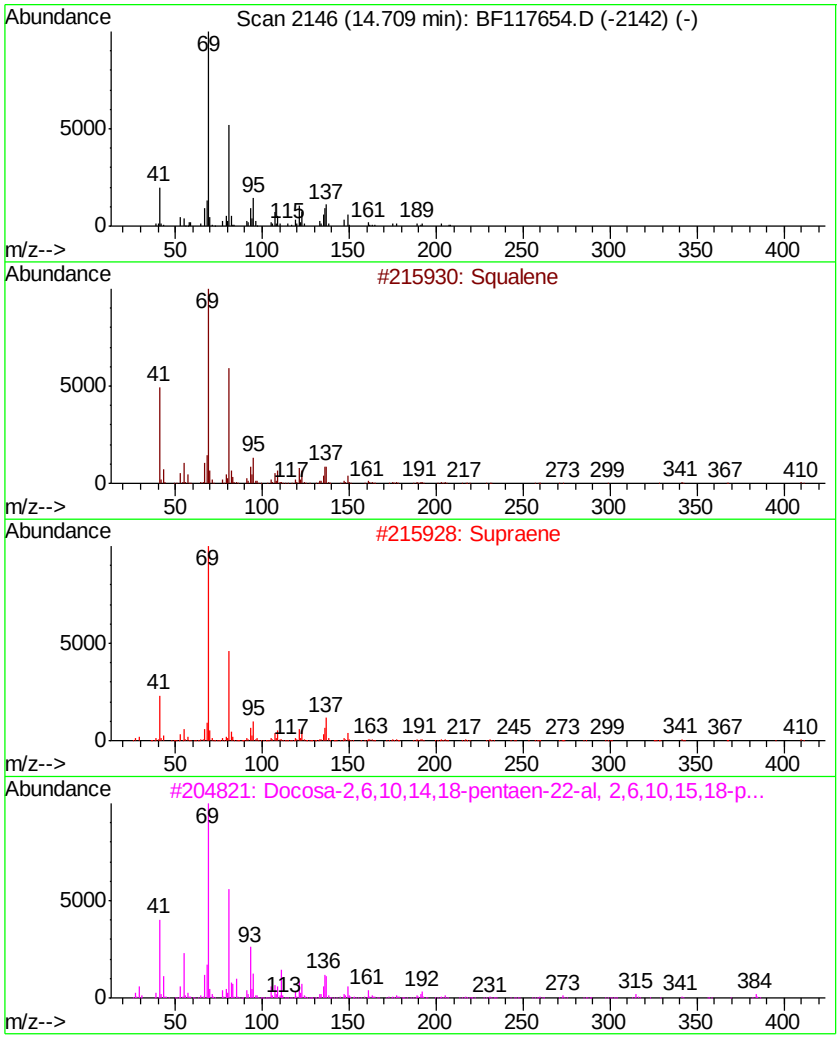
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

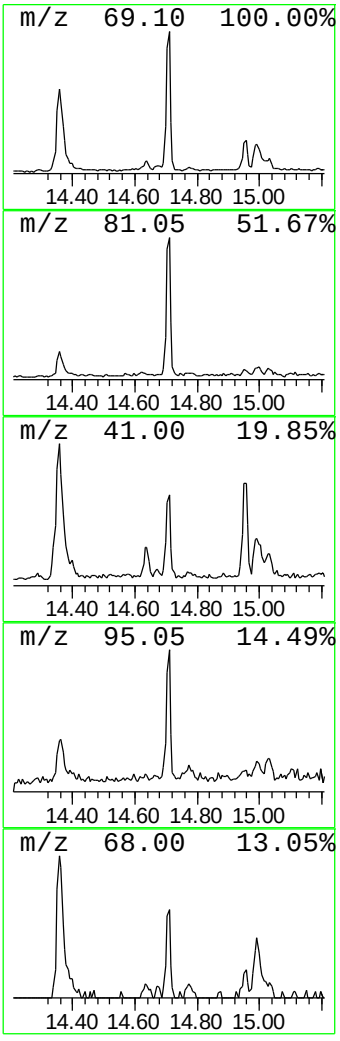
****

Peak Number 10 Squalene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	14.91 ng	138897	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	74
5	Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

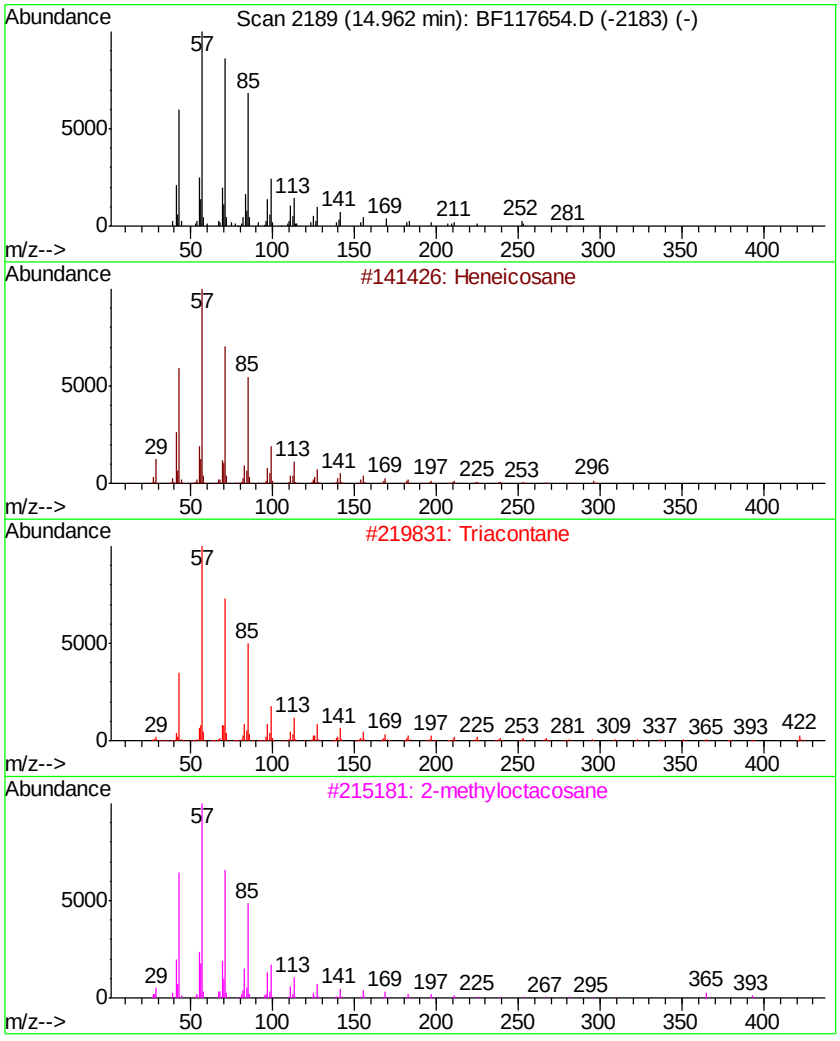
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

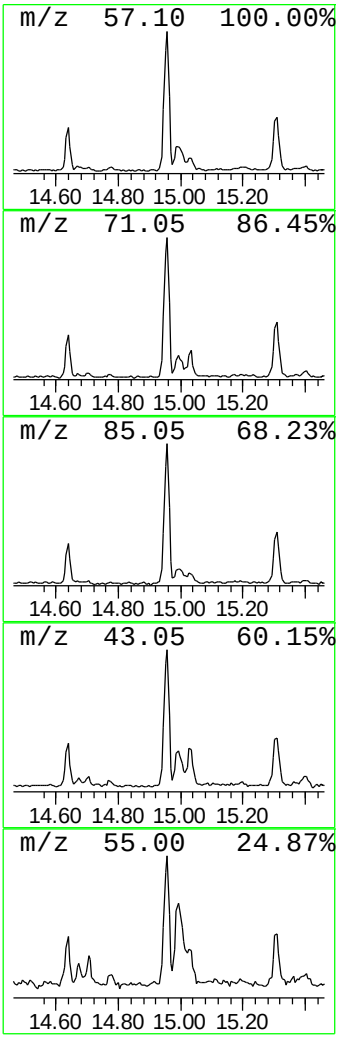
****

Peak Number 11 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	29.81 ng	277654	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Triacontane	422	C30H62	000638-68-6	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	90
5	Heptadecane	240	C17H36	000629-78-7	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

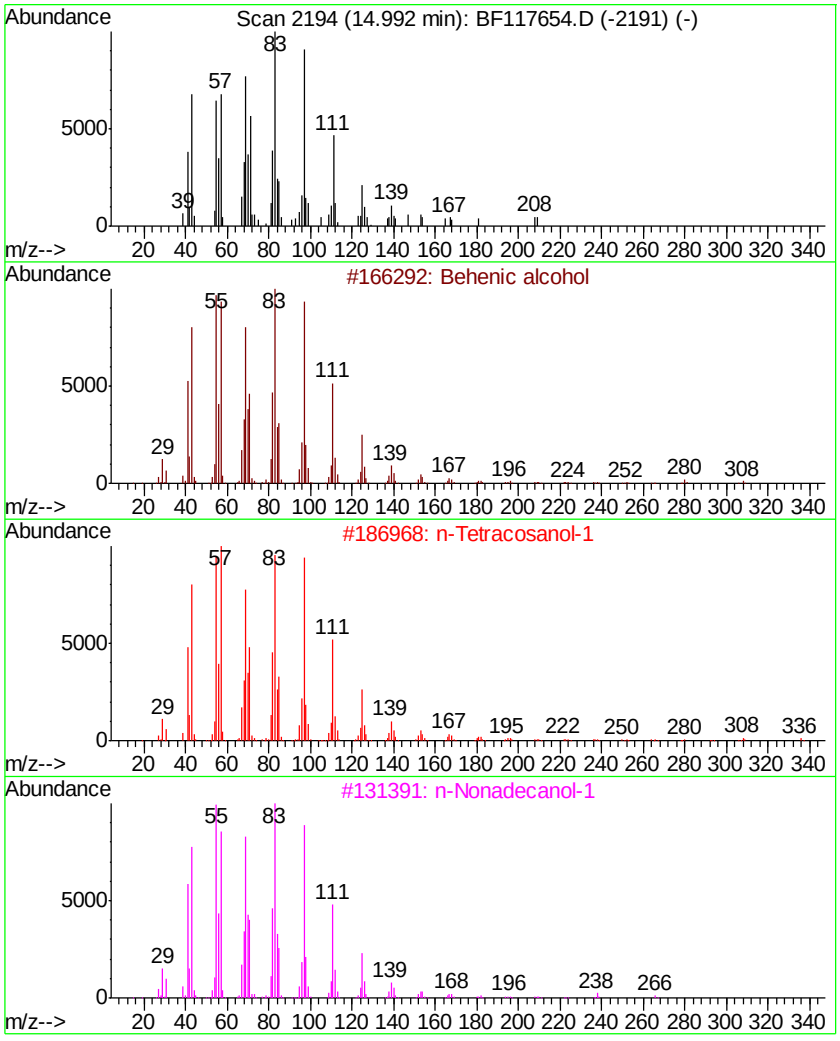
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

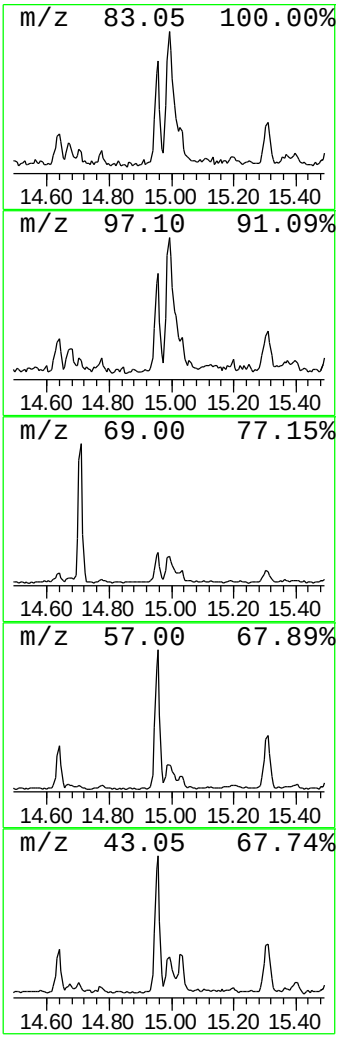
****

Peak Number 12 n-Tetracosanol-1 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	17.23 ng	160434	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	87
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	70
4	1-Docosene	308	C22H44	001599-67-3	60
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	60





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

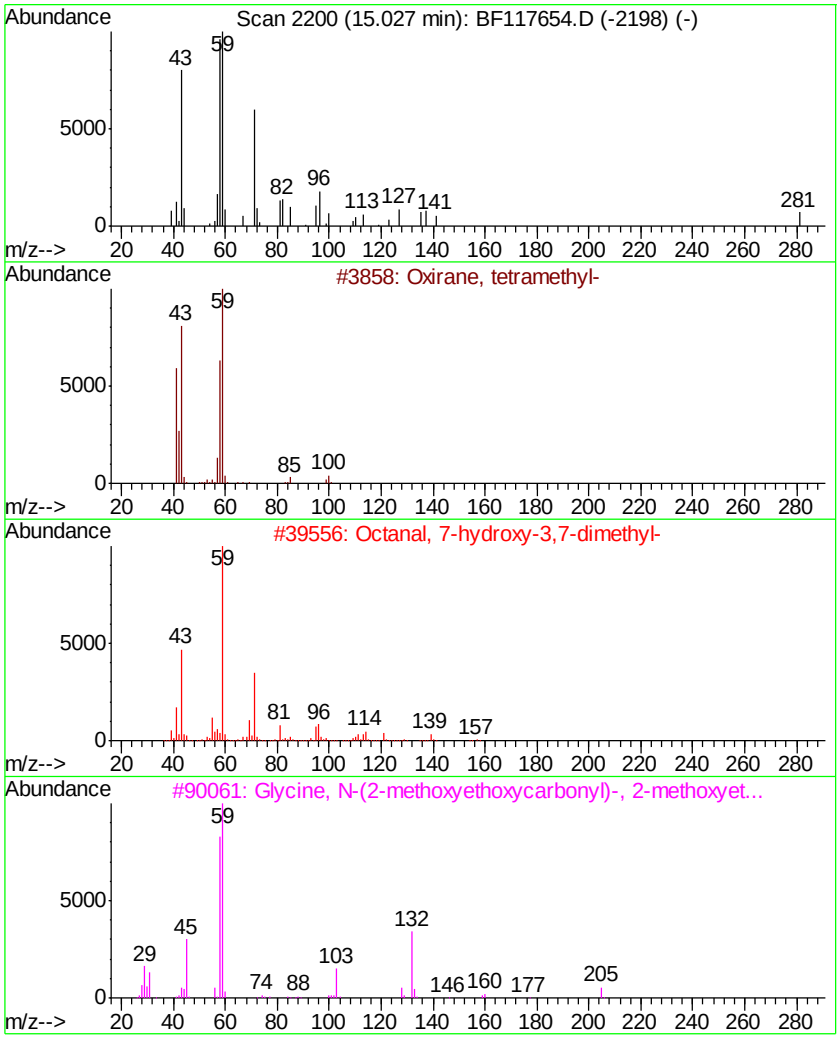
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

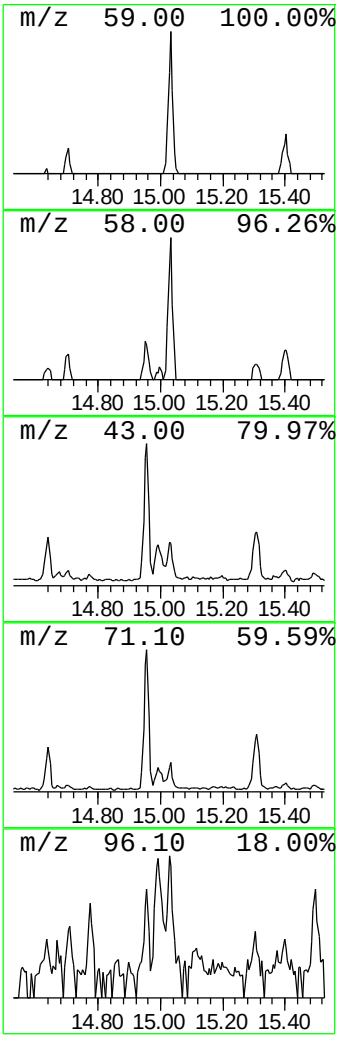
****

Peak Number 13 Oxirane, tetramethyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	8.42 ng	78467	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	50
2	Octanal, 7-hydroxy-3,7-dimethyl-	172	C10H20O2	000107-75-5	37
3	Glycine, N-(2-methoxyethoxycarbo...	235	C9H17NO6	1000328-06-4	33
4	d-Ribo-tetrofuranose, 4-c-cyclop...	200	C10H16O4	030571-50-7	32
5	2H-Pyran,3,4-dihydro-2-methoxy-4...	128	C7H12O2	038113-08-5	27





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

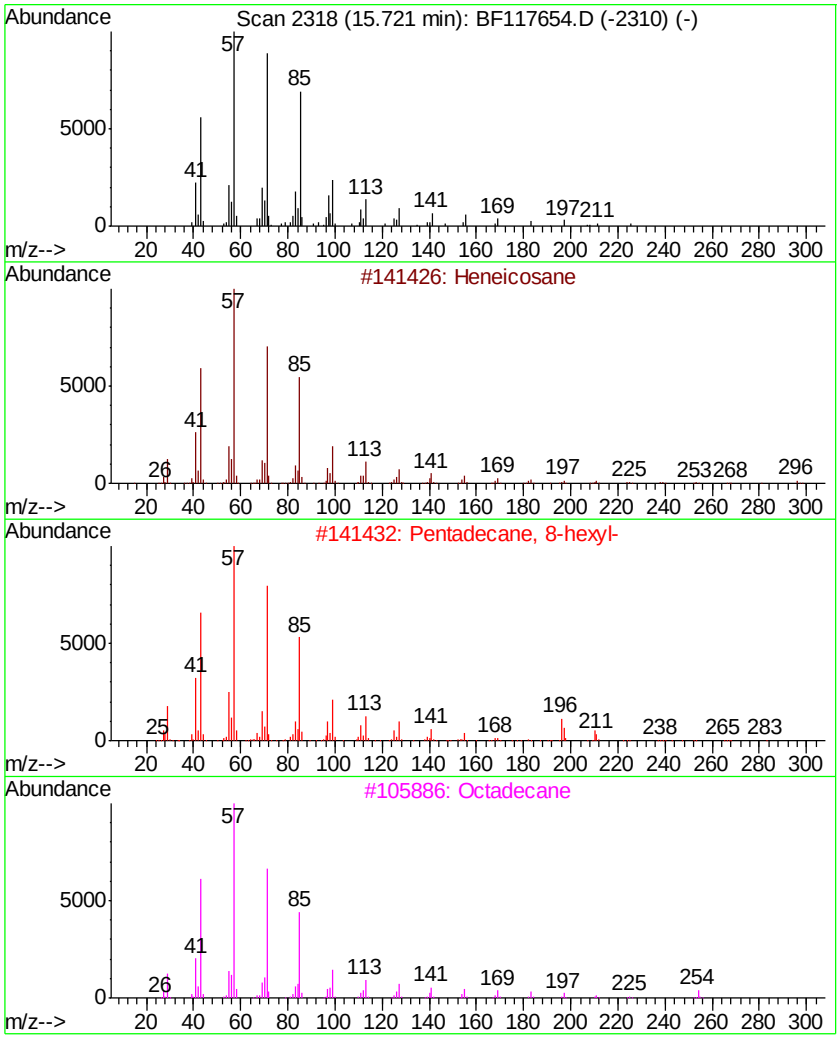
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

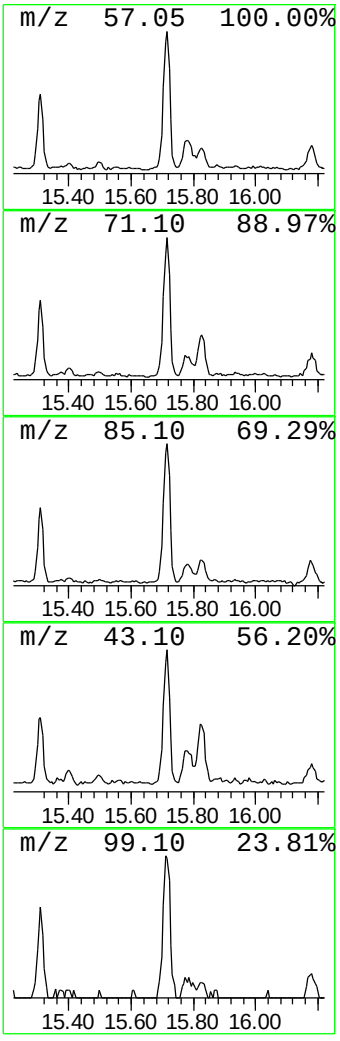
****

Peak Number 14 Pentadecane, 8-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	27.83 ng	259214	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

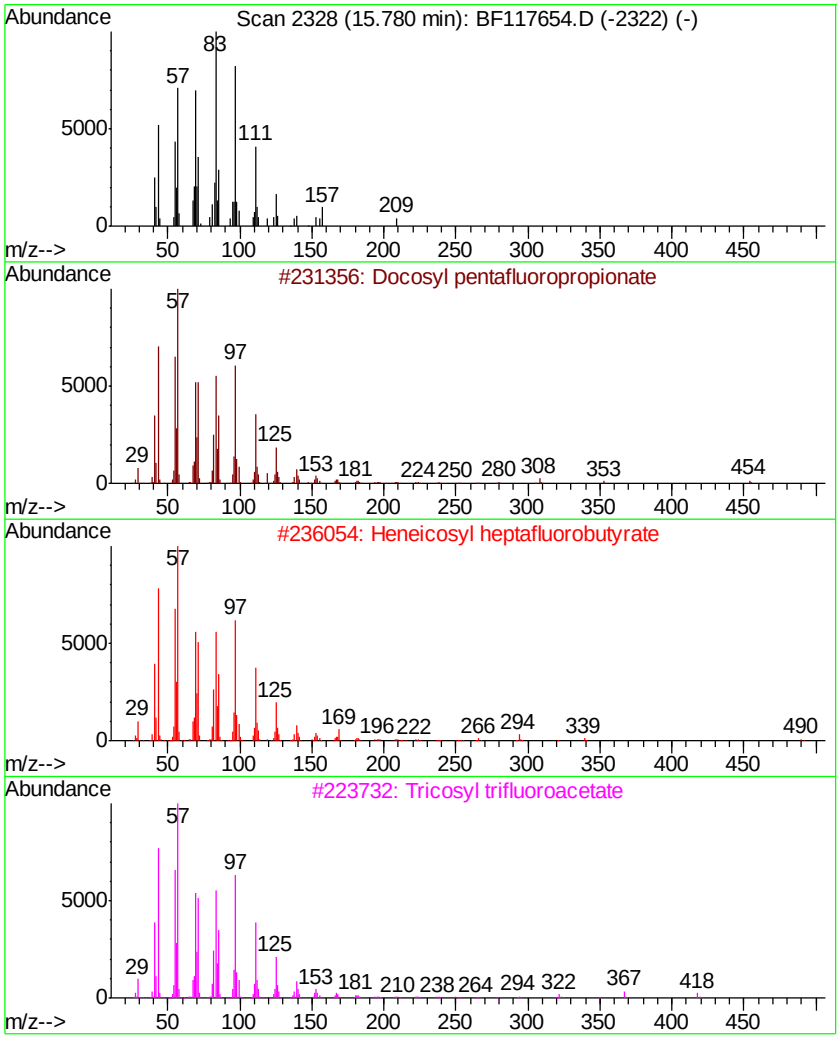
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

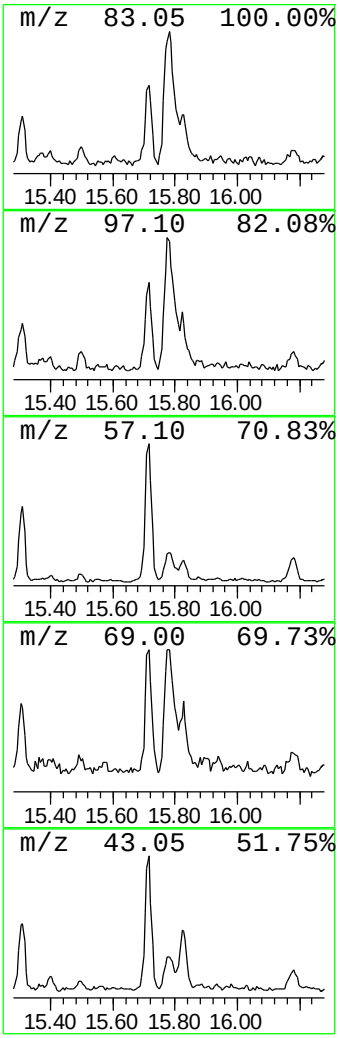
****

Peak Number 15 Docosyl pentafluoropropionate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	16.28 ng	151668	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	50
2	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	50
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	50
4	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	50
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

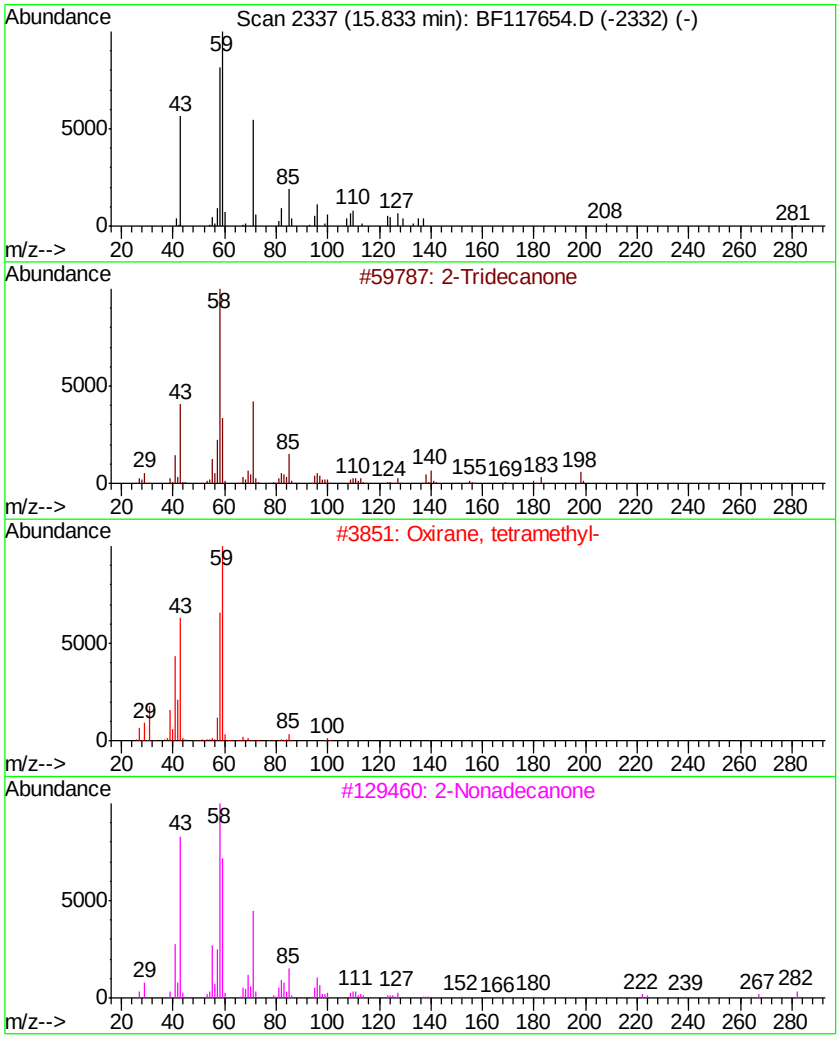
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

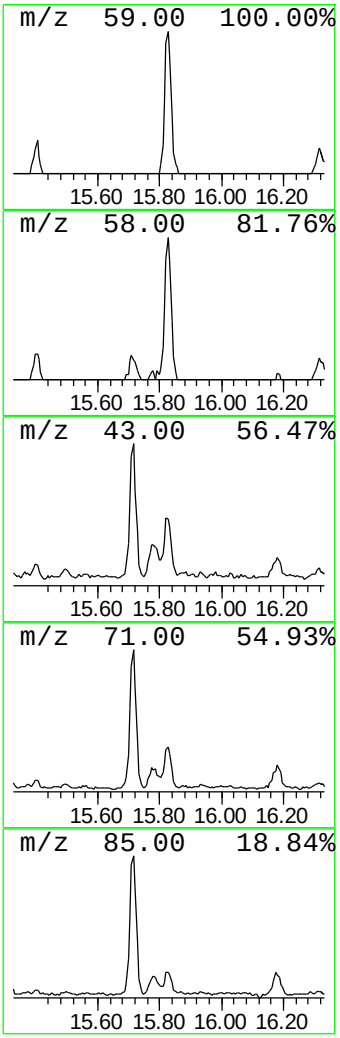
****

Peak Number 16 2-Tridecanone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	14.10 ng	131319	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Tridecanone	198	C13H26O	000593-08-8	53
2	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	49
3	2-Nonadecanone	282	C19H38O	000629-66-3	45
4	Octanal, 7-hydroxy-3,7-dimethyl-	172	C10H20O2	000107-75-5	38
5	Undecanal, 2-methyl-	184	C12H24O	000110-41-8	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

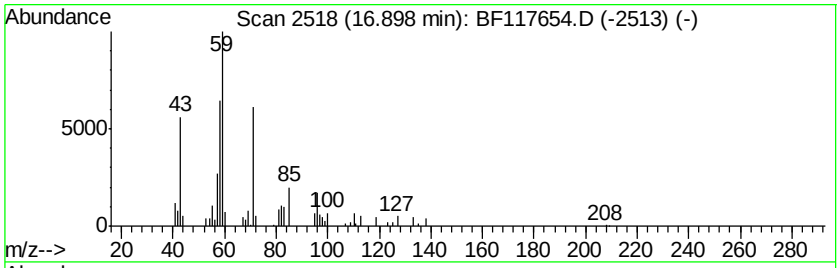
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

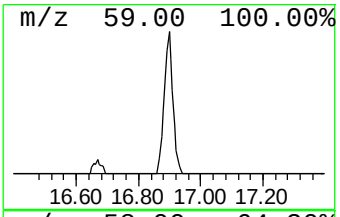
****

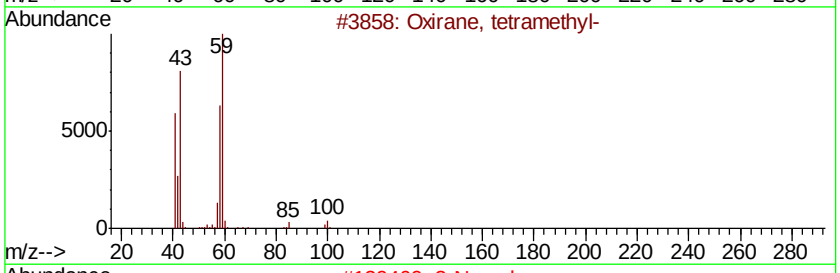
Peak Number 17 unknown16.90 Concentration Rank 16

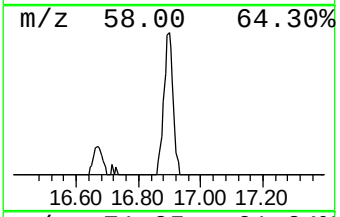
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.90	13.32 ng	124011	Perylene-d12	15.34

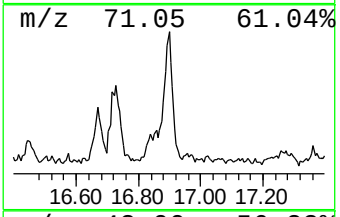
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	46
2	2-Nonadecanone	282	C19H38O	000629-66-3	45
3	2-Tridecanone	198	C13H26O	000593-08-8	38
4	Hexane, 1-(ethoxymethoxy)-	160	C9H20O2	151705-35-0	32
5	Oxirane, 2,3-diethyl-	100	C6H12O	004468-66-0	27

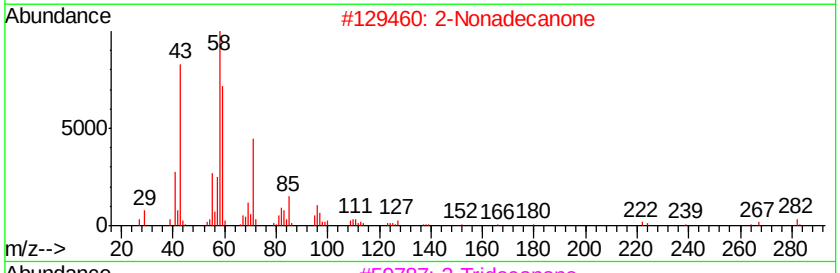


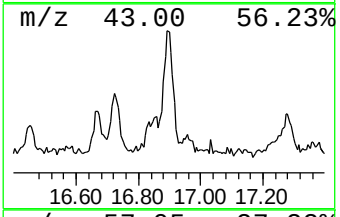


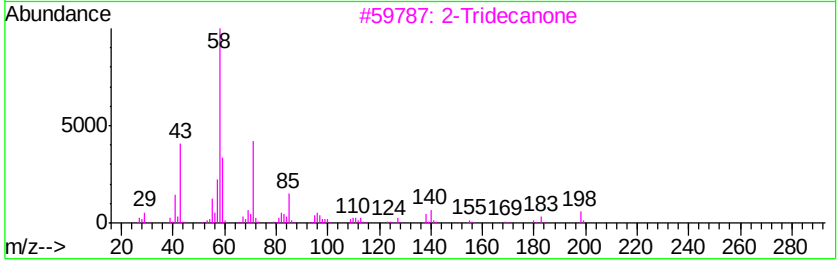


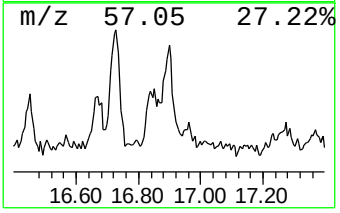












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

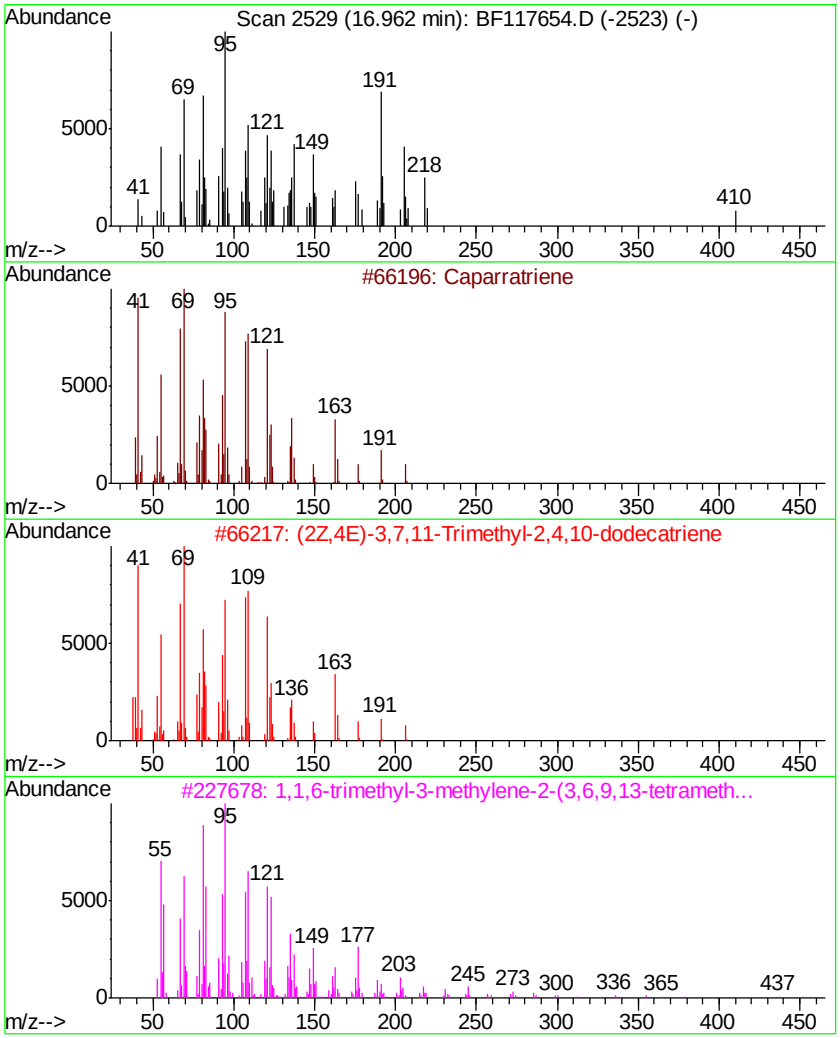
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

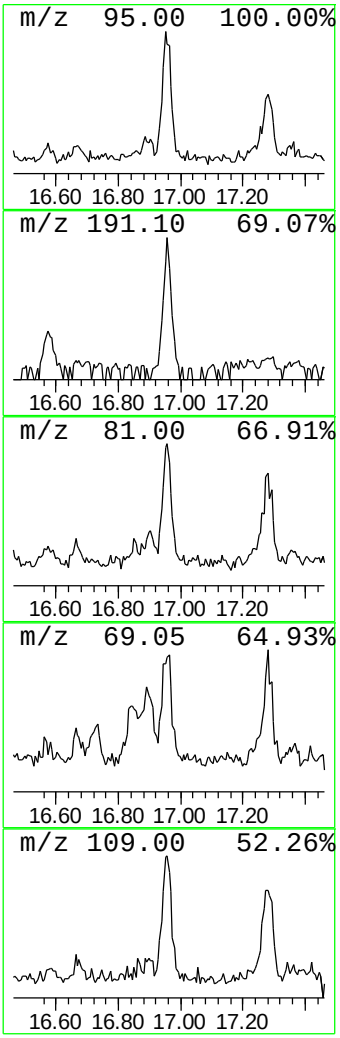
****

Peak Number 18 Caparratriene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	16.27 ng	151506	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caparratriene	206	C15H26	1000374-08-7	91
2	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	60
3	1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	53
4	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	35
5	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

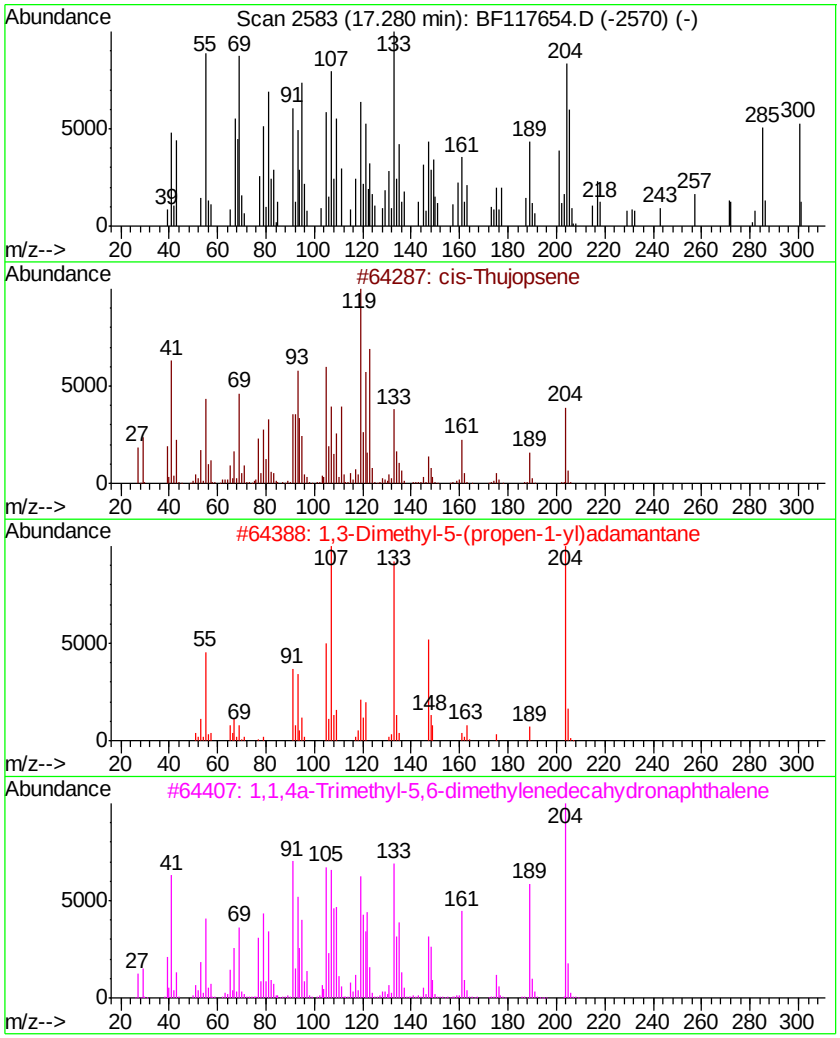
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

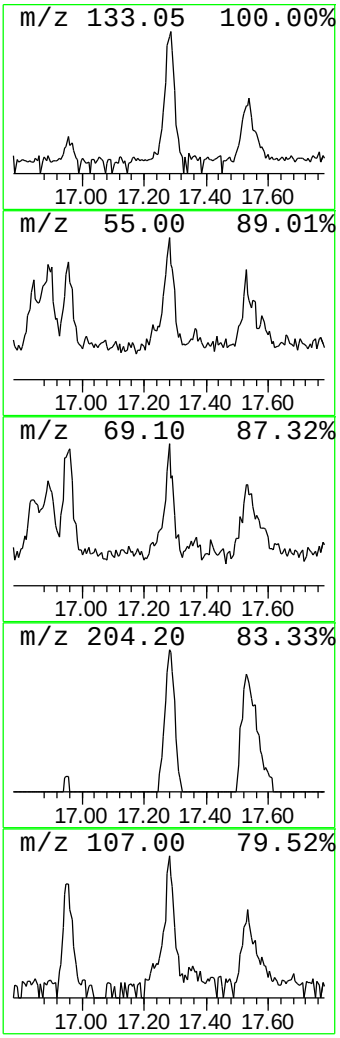
****

Peak Number 19 cis-Thujopsene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.28	26.35 ng	245452	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Thujopsene	204	C15H24	000470-40-6	52
2	1,3-Dimethyl-5-(propen-1-yl)adam...	204	C15H24	057040-48-9	46
3	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	45
4	.gamma.-HIMACHALENE	204	C15H24	1000140-08-0	43
5	Pregna-5,17(20)-dien-3-ol, (3.be...	300	C21H32O	001159-25-7	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

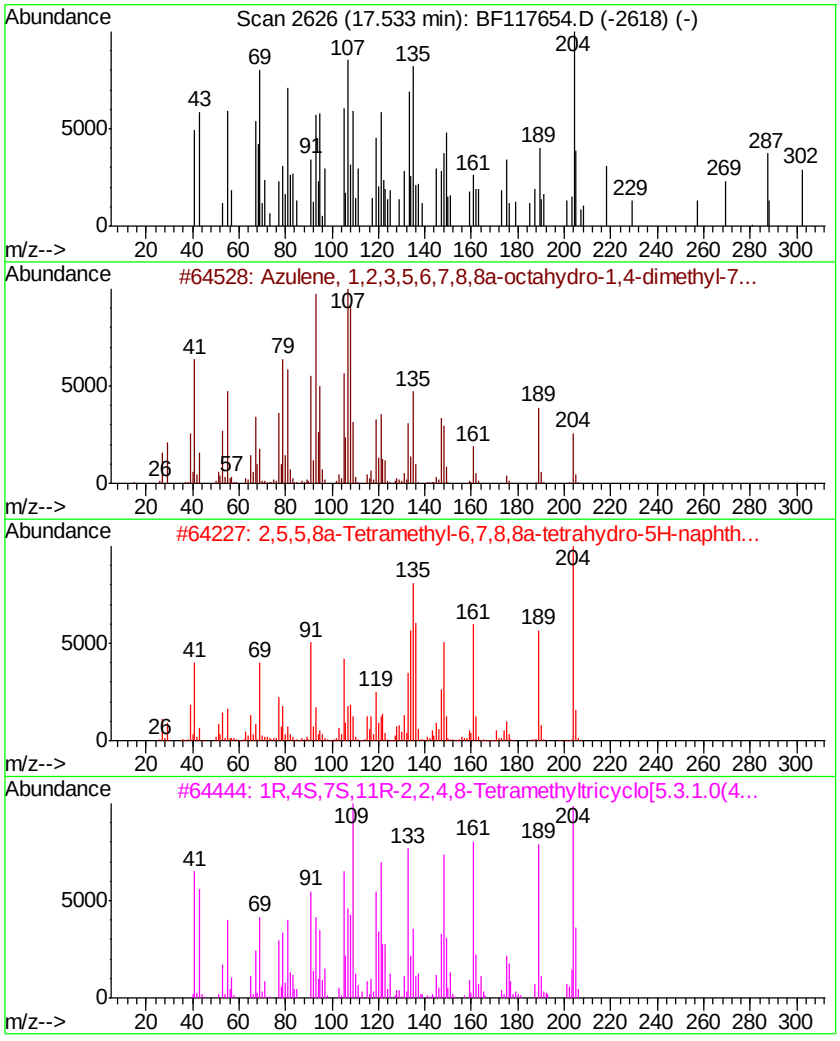
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

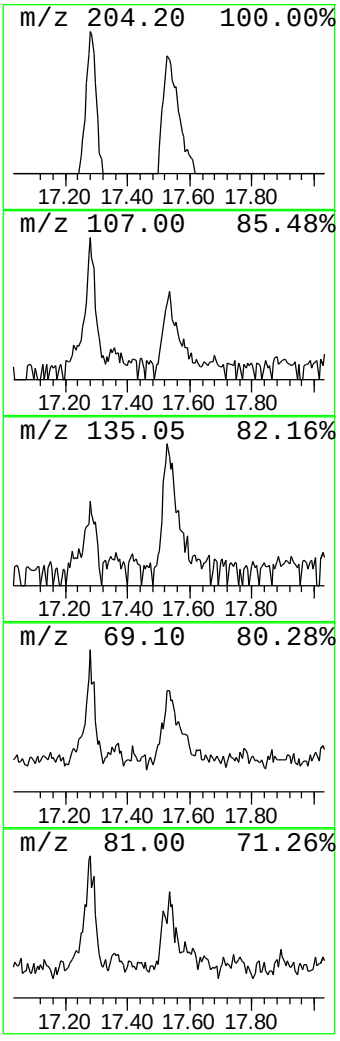
****

Peak Number 20 Azulene, 1,2,3,5,6,7,8,8a-o... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.53	25.09 ng	233702	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azulene, 1,2,3,5,6,7,8,8a-octahv...	204	C15H24	003691-11-0	60
2	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	43
3	1R,4S,7S,11R-2,2,4,8-Tetramethyl...	204	C15H24	1000140-07-6	43
4	1H-Cyclopropa[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	43
5	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103119\
Data File : BF117654.D
Acq On : 31 Oct 2019 13:31
Operator : JU
Sample : K5541-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 153-08-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
unknown6.50	6.50	74.6	ng	694725	1	6.73	186320	20.0
n-Hexadecanoic acid	11.78	7.3	ng	94395	4	11.25	259072	20.0
1-Decanol, 2-hexyl-	13.05	8.3	ng	79102	5	13.90	191596	20.0
2-Phenanthrenol, ...	13.26	23.3	ng	223582	5	13.90	191596	20.0
3-Methoxy-5-napht...	13.29	18.5	ng	177649	5	13.90	191596	20.0
Trichloroacetic a...	13.72	40.4	ng	387401	5	13.90	191596	20.0
Behenic alcohol	14.36	55.6	ng	532434	5	13.90	191596	20.0
2-methyloctacosane	14.64	8.8	ng	81923	6	15.34	186272	20.0
Squalene	14.71	14.9	ng	138897	6	15.34	186272	20.0
Heneicosane	14.96	29.8	ng	277654	6	15.34	186272	20.0
n-Tetracosanol-1	14.99	17.2	ng	160434	6	15.34	186272	20.0
Oxirane, tetramet...	15.03	8.4	ng	78467	6	15.34	186272	20.0
Pentadecane, 8-he...	15.72	27.8	ng	259214	6	15.34	186272	20.0
Docosyl pentafluo...	15.78	16.3	ng	151668	6	15.34	186272	20.0
2-Tridecanone	15.83	14.1	ng	131319	6	15.34	186272	20.0
unknown16.90	16.90	13.3	ng	124011	6	15.34	186272	20.0
Caparratriene	16.96	16.3	ng	151506	6	15.34	186272	20.0
cis-Thujopsene	17.28	26.4	ng	245452	6	15.34	186272	20.0
Azulene, 1,2,3,5,...	17.53	25.1	ng	233702	6	15.34	186272	20.0