LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

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-BF051019.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	2.128	3	7	24	rVB	1334145	1933019	14.33%	1.538%
2	5.498	575	580	590	rBV	6120919	6555774	48.62%	5.215%
3	6.516	747	753	763	rBV	5917065	7099911	52.65%	5.648%
4	6.640	769	774	777	rBV	6728305	6751353	50.07%	5.370%
5	6.857	807	811	814	rBV	1956714	1633299	12.11%	1.299%
6	7.016	833	838	841	rBV	5788952	5218317	38.70%	4.151%
7	7.422	901	907	910	rBV	4603105	4663632	34.58%	3.710%
8	8.134	1022	1028	1032	rBV	2189184	2048598	15.19%	1.630%
9	9.210	1206	1211	1214	rBV	6872711	6383690	47.34%	5.078%
10	9.604	1274	1278	1287	rVB	1045341	1078801	8.00%	0.858%
11	9.892	1323	1327	1337	rVB	2424099	2235421	16.58%	1.778%
12	10.686	1457	1462	1465	rBV	4206191	4154309	30.81%	3.305%
13	10.916	1496	1501	1505	rVB2	226352	233621	1.73%	0.186%
14	11.039	1518	1522	1525	rBV2	209372	250408	1.86%	0.199%
15	11.075	1525	1528	1533	rVB2	180305	158816	1.18%	0.126%
16	11.327	1567	1571	1572	rBV2	135023	156288	1.16%	0.124%
17	11.380	1576	1580	1582	rVV	2213353	2231493	16.55%	1.775%
18	11.398	1582	1583	1585	rVV	254157	225764	1.67%	0.180%
19	11.422	1585	1587	1590	rVV2	382749	433795	3.22%	0.345%
20	11.480	1594	1597	1599	rVV2	156893	166267	1.23%	0.132%
21	11.527	1602	1605	1609	rVV2	174930	189807	1.41%	0.151%
22	11.592	1613	1616	1622	rVV	257845	304147	2.26%	0.242%
23	11.651	1623	1626	1633	rVB3	94717	160826	1.19%	0.128%
24	11.739	1638	1641	1649	rVB4	111660	217153	1.61%	0.173%
25	11.904	1665	1669	1676	rBV	1561694	1564732	11.60%	1.245%
26	12.069	1695	1697	1703	rVB2	124264	168094	1.25%	0.134%
27	12.233	1722	1725	1728	rBV	171303	167002	1.24%	0.133%
28	12.416	1752	1756	1759	rBV3	158891	205552	1.52%	0.164%
29	12.457	1760	1763	1766	rVV	312684	274080	2.03%	0.218%
30	12.504	1766	1771	1778	rVB2	316275	445177	3.30%	0.354%
31	12.592	1783	1786	1790	rBV	212884	305636	2.27%	0.243%
32	12.639	1791	1794	1796	rVB	326751	307773	2.28%	0.245%
33	12.686	1799	1802	1806	rBV	465025	475185	3.52%	0.378%
34	12.827	1822	1826	1828	rBV2	199392	236490	1.75%	0.188%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

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-BF051019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.963	1844	1849	1852	rVB	4556137	4434448	32.88%	3.527%
36	13.145	1877	1880	1881	rBV	460673	415238	3.08%	0.330%
37	13.163	1881	1883	1885	rVV	603328	620773	4.60%	0.494%
38	13.186	1885	1887	1890	rVB	914045	718323	5.33%	0.571%
39	13.333	1909	1912	1915	rVB	550050	432738	3.21%	0.344%
40	13.404	1921	1924	1926	rBV	203129	174895	1.30%	0.139%
41	13.433	1926	1929	1932	rVV3	369332	371797	2.76%	0.296%
42	13.527	1939	1945	1947	rBV4	480983	837645	6.21%	0.666%
43	13.645	1962	1965	1969	rBV3	457841	499048	3.70%	0.397%
44	13.780	1971	1988	1990	rBV3	1555601	5489591	40.71%	4.367%
45	13.857	1997	2001	2019	rVB2	5717149	13484896	100.00%	10.727%
46	13.980	2019	2022	2025	rBV	250325	254067	1.88%	0.202%
47	14.021	2026	2029	2032	rVV	1567950	1680249	12.46%	1.337%
48	14.051	2032	2034	2037	rVV	517747	401955	2.98%	0.320%
49	14.080	2037	2039	2043	rVB	207521	175205	1.30%	0.139%
50	14.180	2053	2056	2058	rBV	650809	680457	5.05%	0.541%
51	14.310	2075	2078	2081	rVB	543891	539480	4.00%	0.429%
52	14.504	2107	2111	2118	rBV	6027090	8513112	63.13%	6.772%
53	14.557	2118	2120	2125	rVV	350175	359630	2.67%	0.286%
54	14.627	2129	2132	2135	rBV	274592	232118	1.72%	0.185%
55	14.721	2146	2148	2151	rBV	229930	317098	2.35%	0.252%
56	14.810	2158	2163	2165	rBV2	644379	937322	6.95%	0.746%
57	14.951	2184	2187	2194	rVB	1029330	1120279	8.31%	0.891%
58	15.151	2217	2221	2224	rBV	3026408	4129712	30.62%	3.285%
59	15.180	2224	2226	2231	rVV	2091187	2415231	17.91%	1.921%
60	15.227	2231	2234	2246	rVV	672087	1280987	9.50%	1.019%
61	15.315	2247	2249	2255	rVB2	391914	462605	3.43%	0.368%
62	15.521	2280	2284	2289	rBV2	1422362	1950258	14.46%	1.551%
63	15.733	2316	2320	2329	rVB	1351766	1993223	14.78%	1.586%
64	15.968	2355	2360	2365	rBV	1754671	2615173	19.39%	2.080%
65	16.021	2365	2369	2376	rVV	805040	1295380	9.61%	1.030%
66	16.086	2377	2380	2385	rVB	776482	1132097	8.40%	0.901%
67	16.139	2386	2389	2396	rVB2	333916	524276	3.89%	0.417%
68	16.209	2398	2401	2404	rBV2	242166	313794	2.33%	0.250%
69	16.768	2491	2496	2503	rVB	853903	1578896	11.71%	1.256%
70	17.068	2544	2547	2553	rVB2	235565	369559	2.74%	0.294%
71	17.251	2573	2578	2584	rBV	736319	1479032	10.97%	1.177%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

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-BF051019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	17.309	2584	2588	2601	rVB3	617144	1405341	10.42%	1.118%
73	17.656	2643	2647	2657	rVB4	621315	1442776	10.70%	1.148%

Sum of corrected areas: 125712934

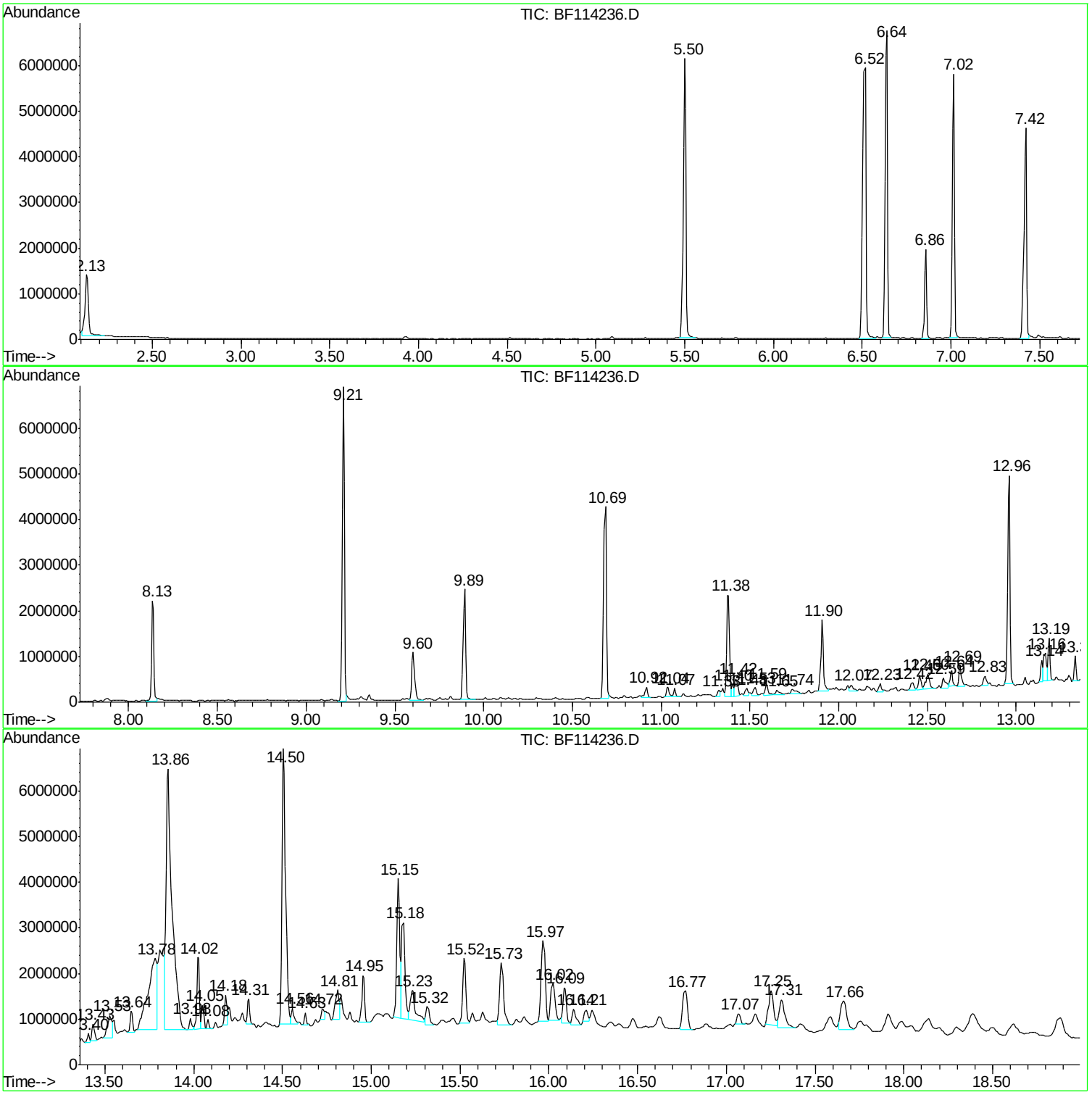
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

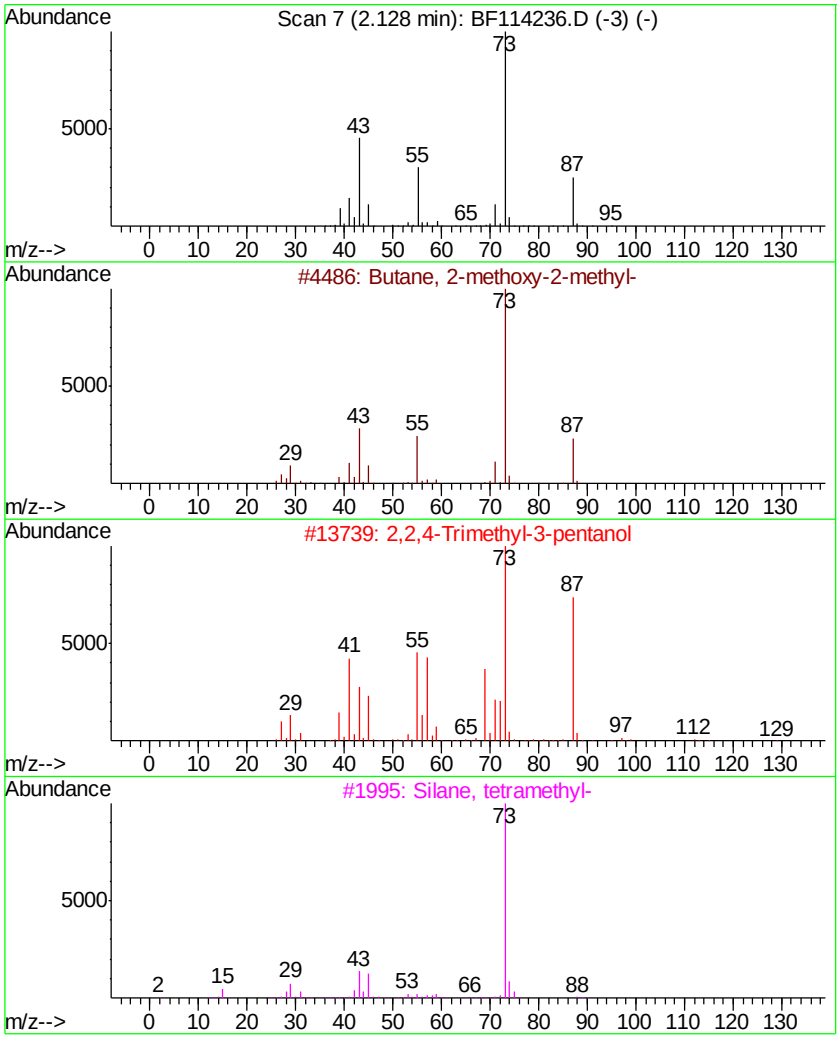
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

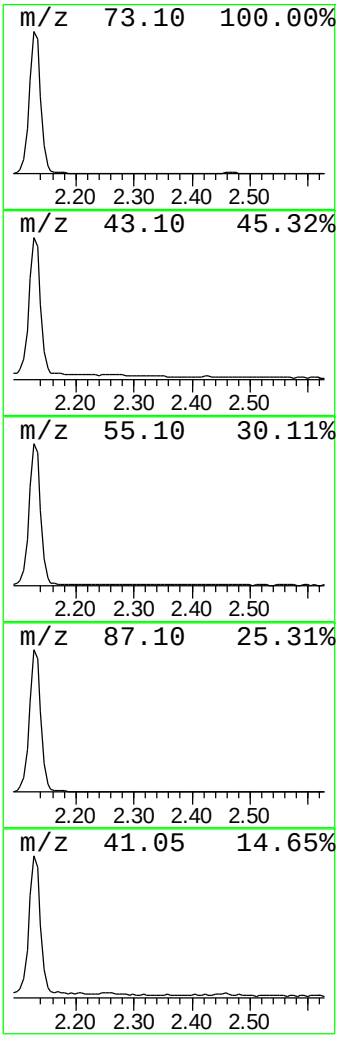
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	23.67 ng	1933020	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

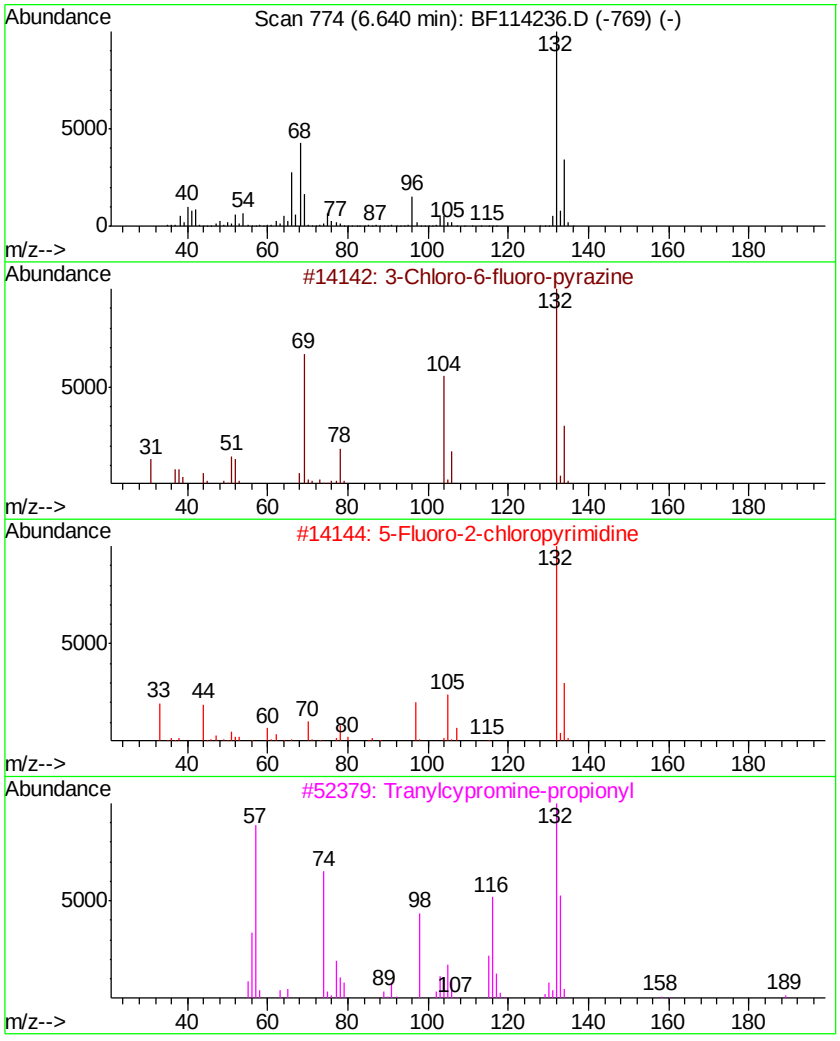
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

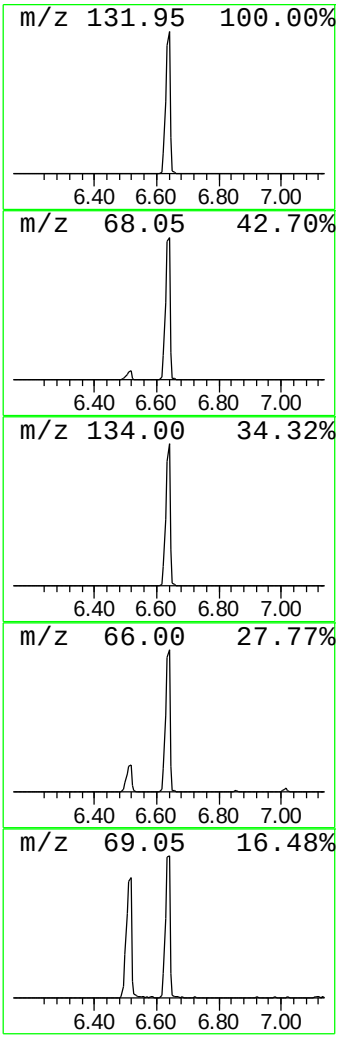
****

Peak Number 2 unknown6.64 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	82.67 ng	6751350	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

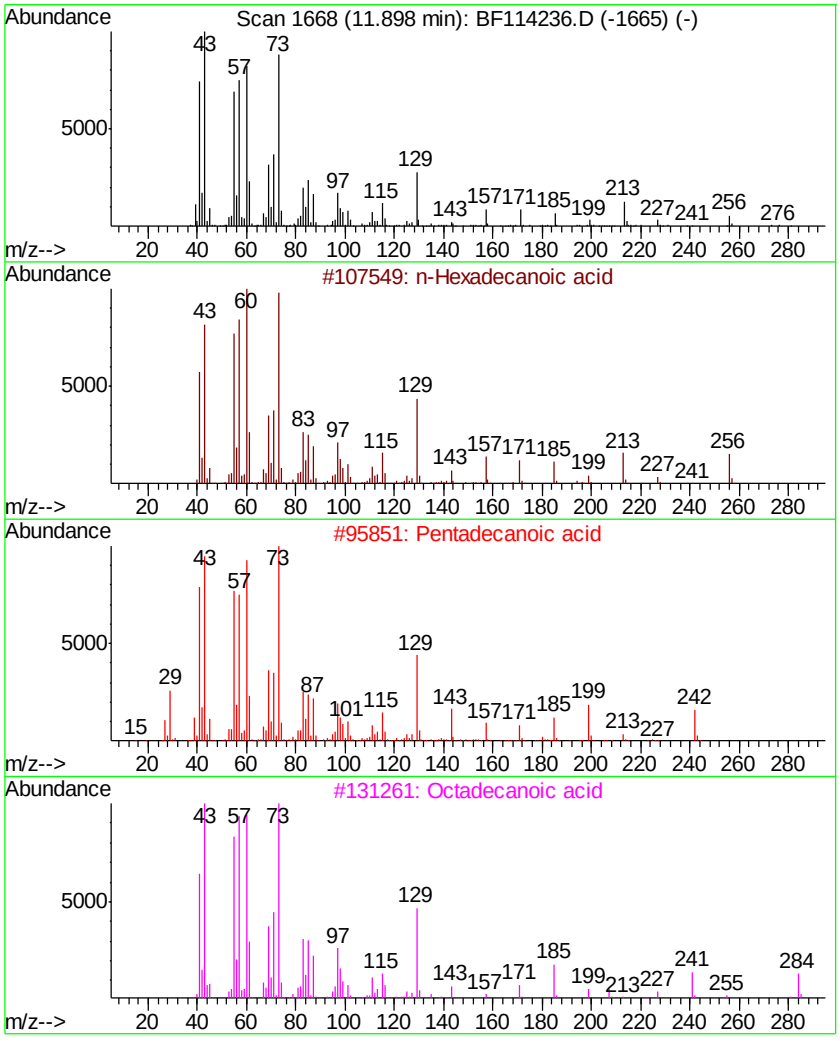
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

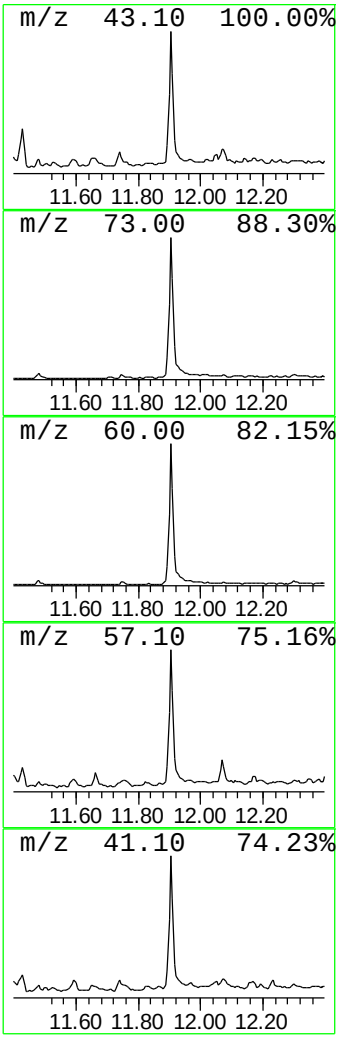
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	14.02 ng	1564730	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

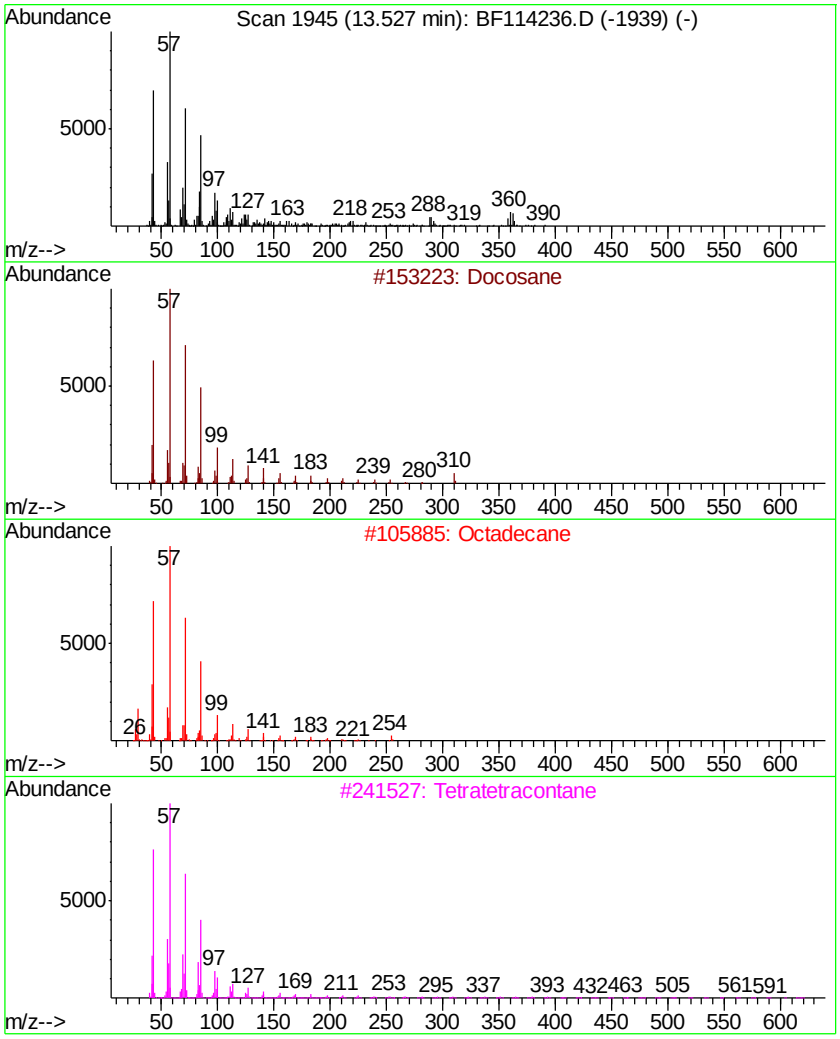
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

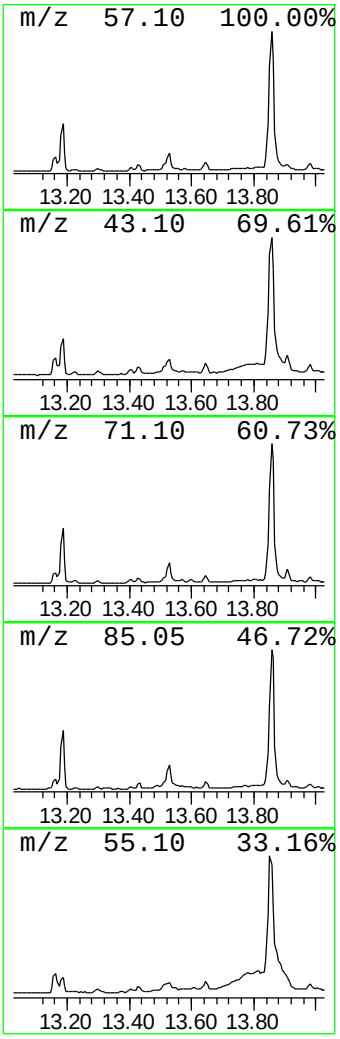
****

Peak Number 5 Docosane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	9.97 ng	837645	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	93
2	Octadecane	254	C18H38	000593-45-3	92
3	Tetratetracontane	619	C44H90	007098-22-8	74
4	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	74
5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	74





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

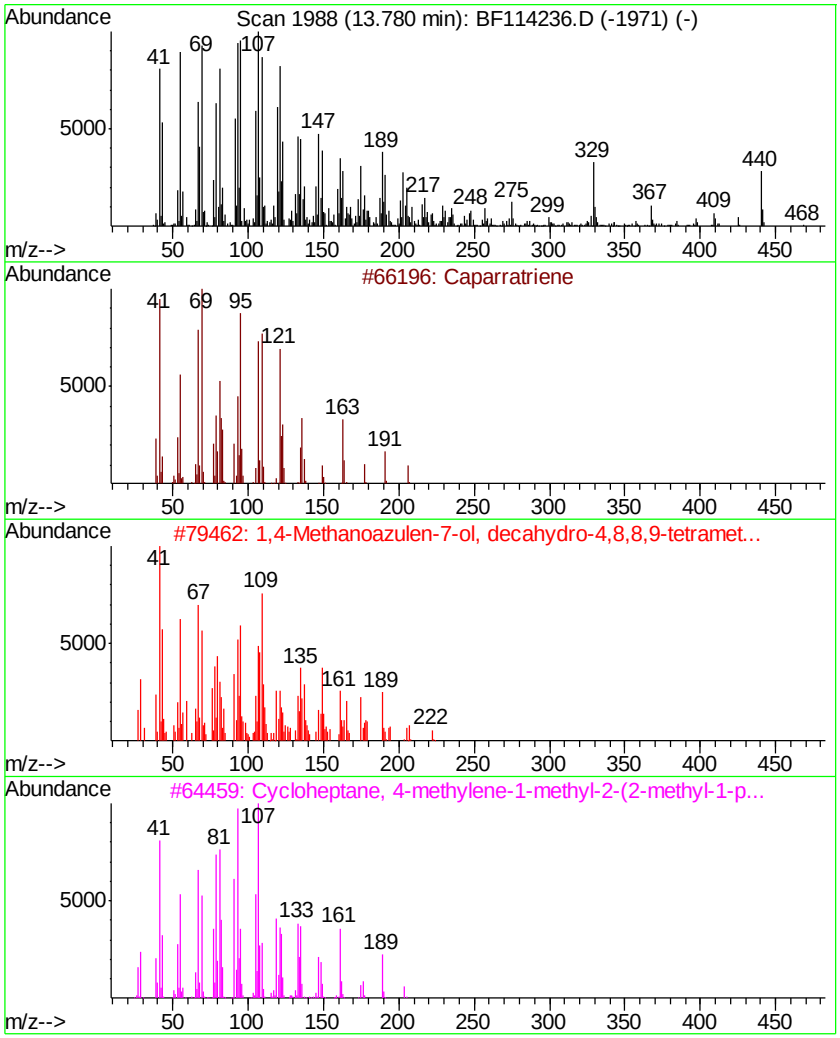
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

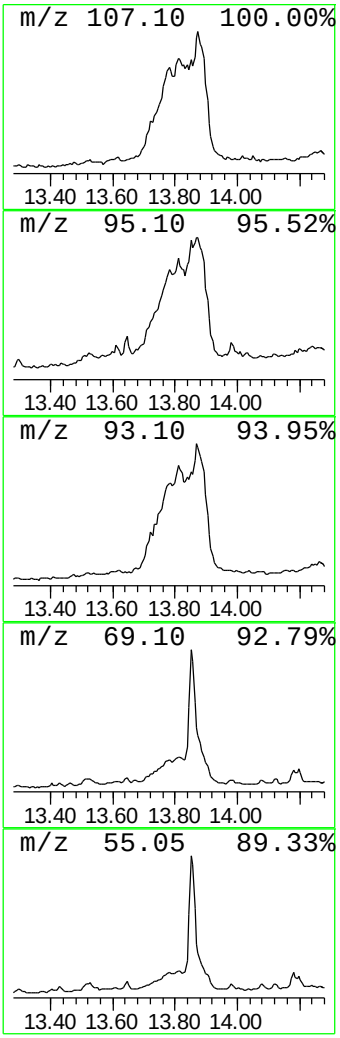
****

Peak Number 6 Caparratriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	65.34 ng	5489590	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caparratriene	206	C15H26	1000374-08-7	58
2	1,4-Methanoazulen-7-ol, decahydr...	222	C15H26O	018319-27-2	45
3	Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	38
4	Ledol	222	C15H26O	000577-27-5	30
5	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	20





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

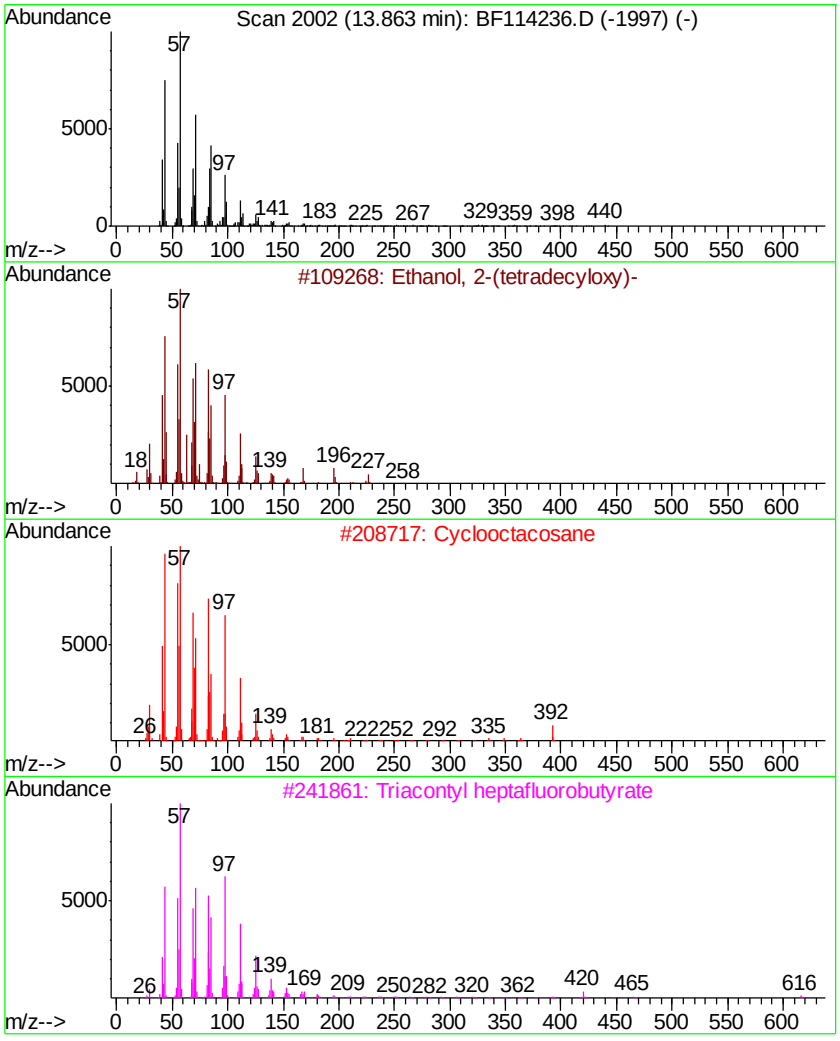
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

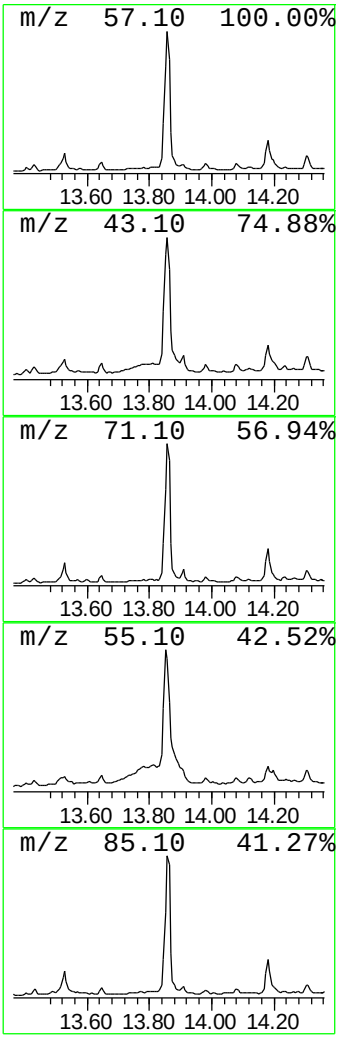
****

Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	160.51 ng	13484900	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	95
2	Cyclooctacosane	392	C28H56	000297-24-5	95
3	Triacontyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	91
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
5	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

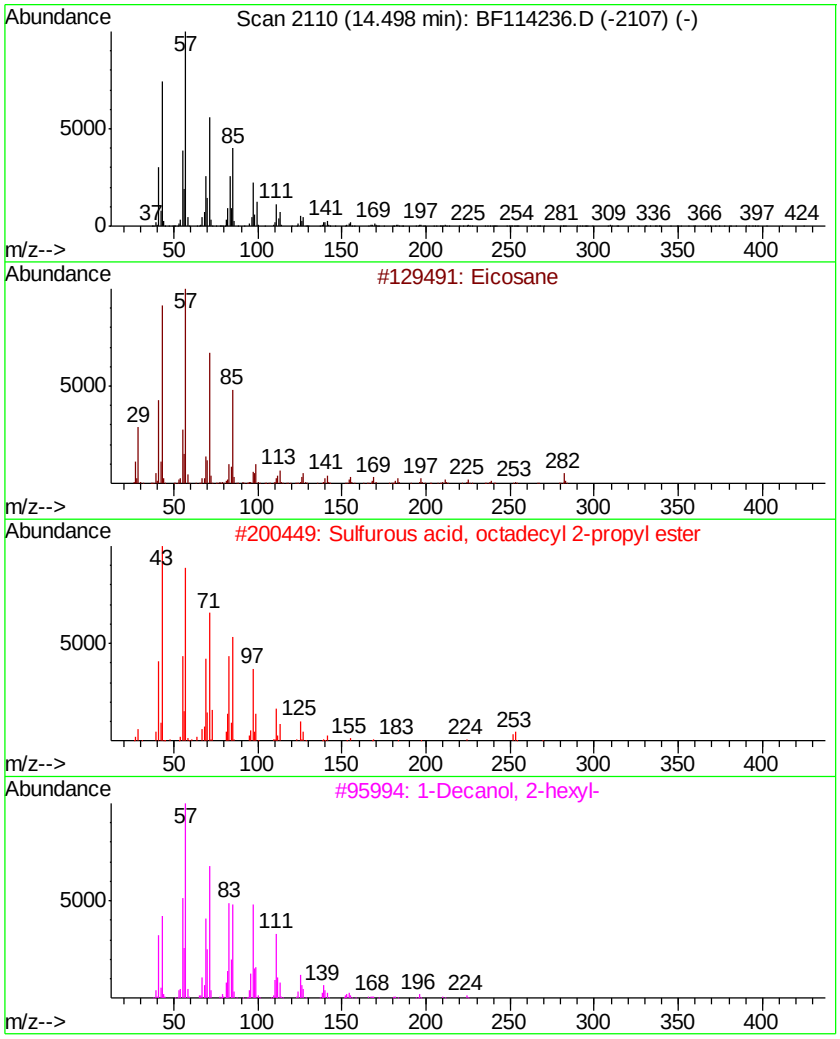
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

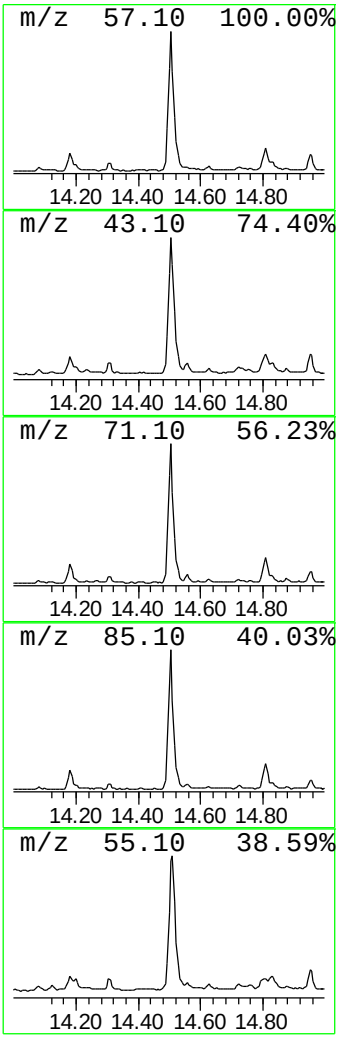
****

Peak Number 8 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	101.33 ng	8513110	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	90
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	81
5	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	74





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

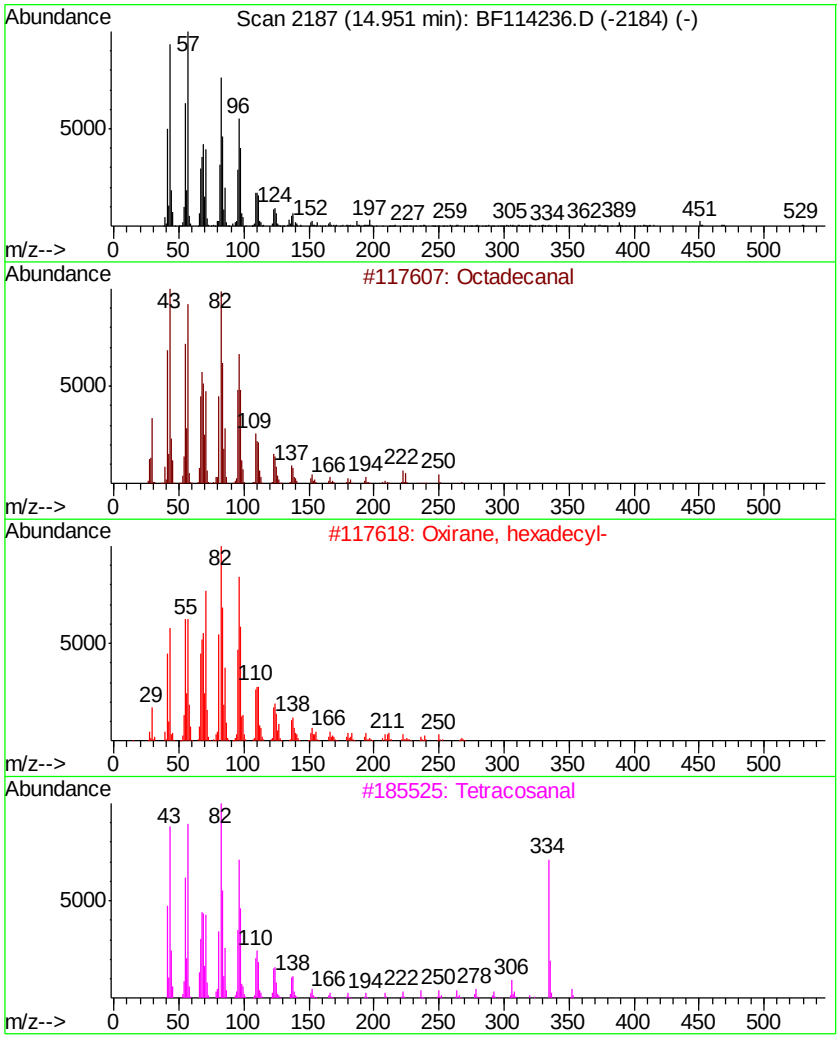
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

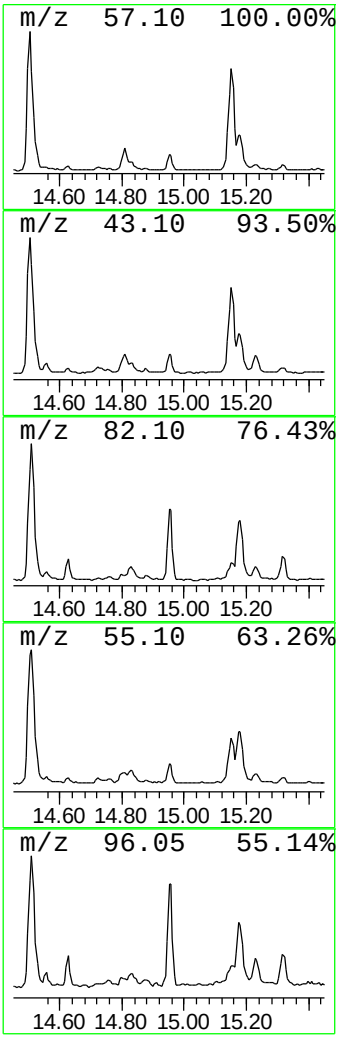
****

Peak Number 9 Octadecanal Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	11.49 ng	1120280	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Tetracosanal	352	C24H48O	057866-08-7	91
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
5	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	89





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

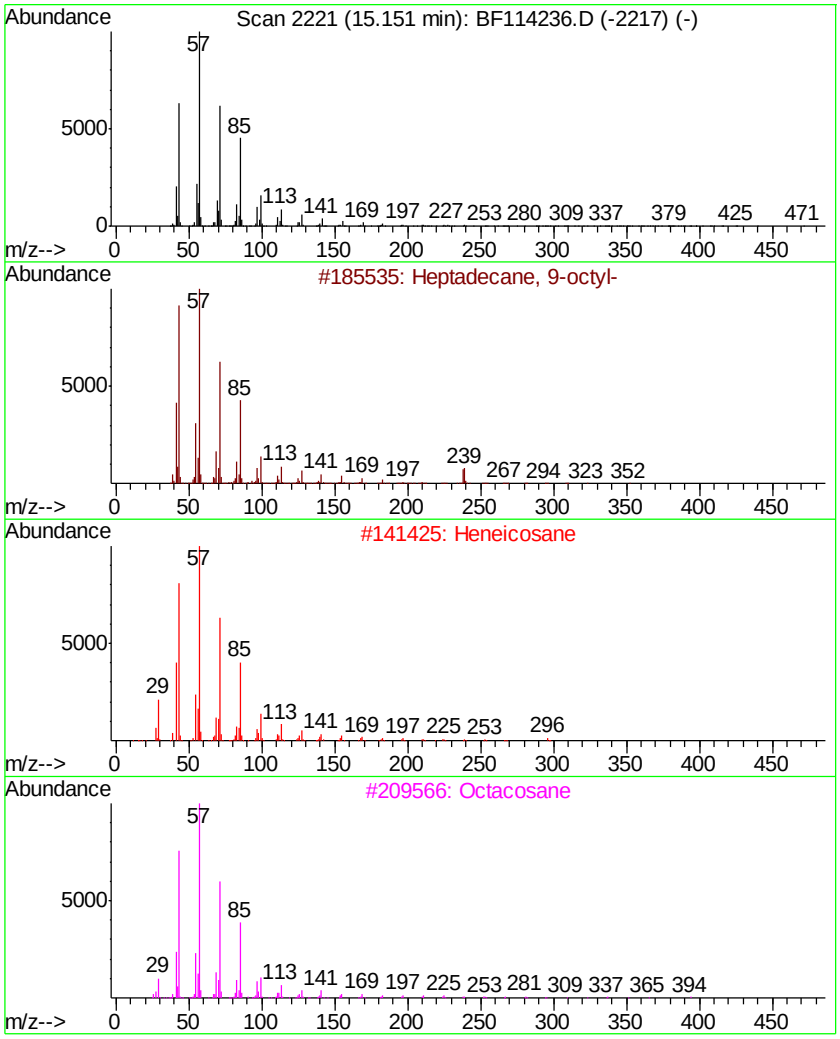
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

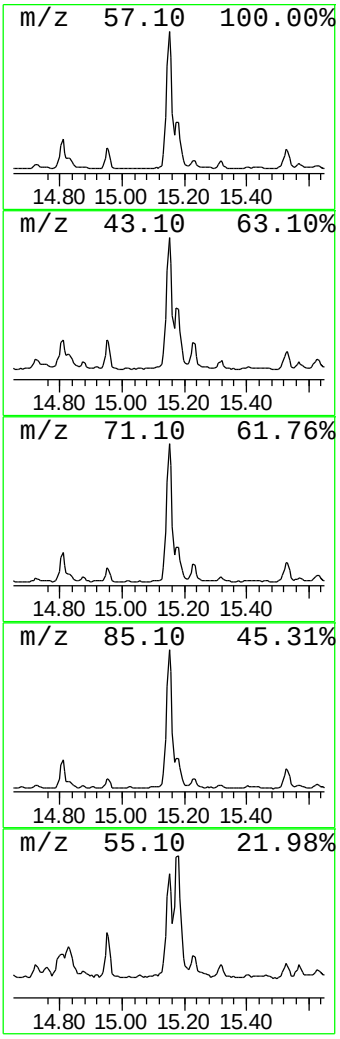
****

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	42.35 ng	4129710	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	96
2	Heneicosane	296	C21H44	000629-94-7	95
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

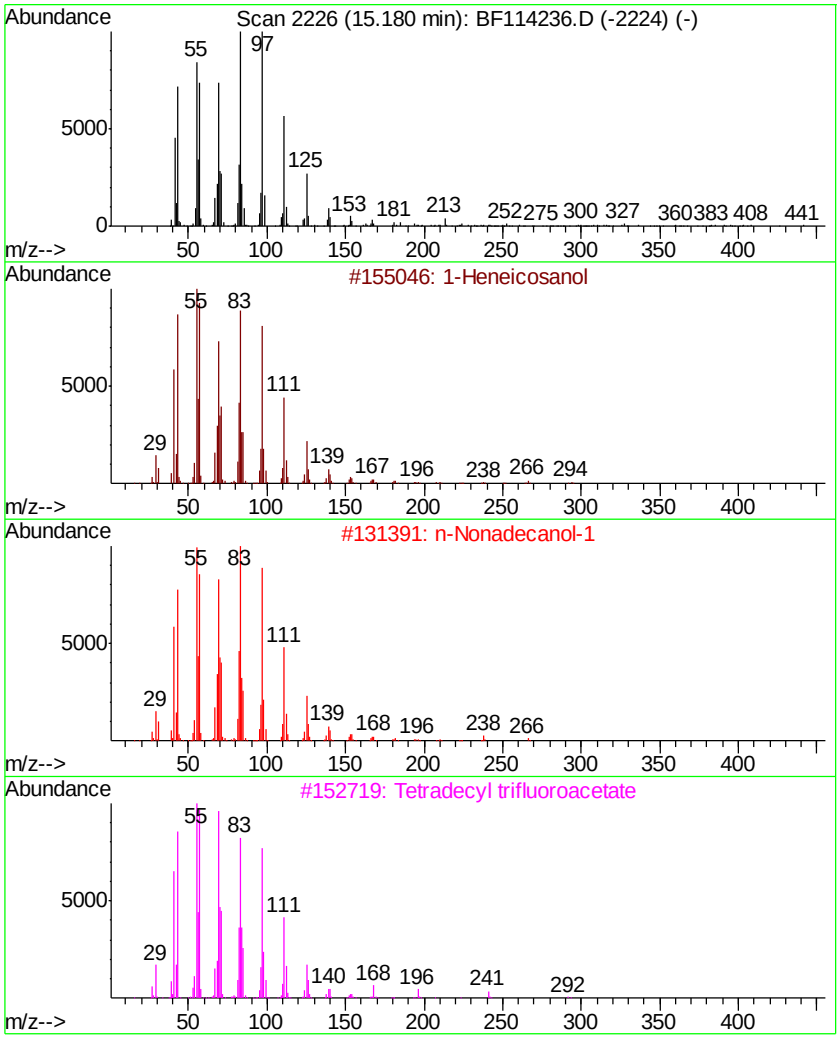
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

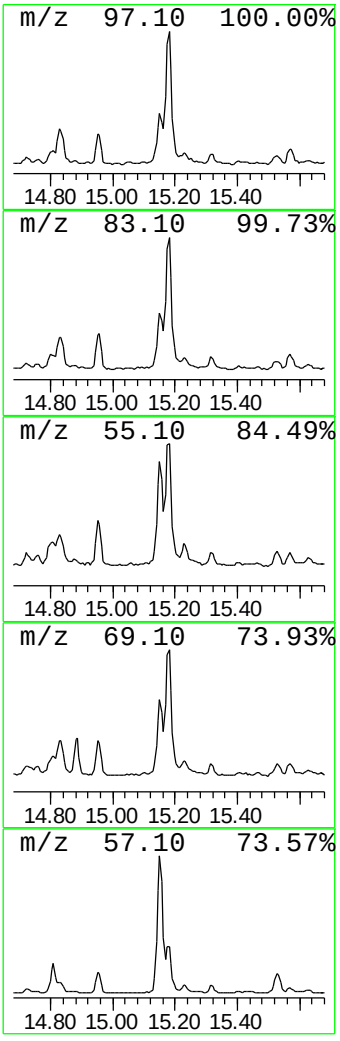
****

Peak Number 11 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	24.77 ng	2415230	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	70
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	64
3	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	58
4	Ergosterol	396	C28H44O	000057-87-4	53
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	52





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

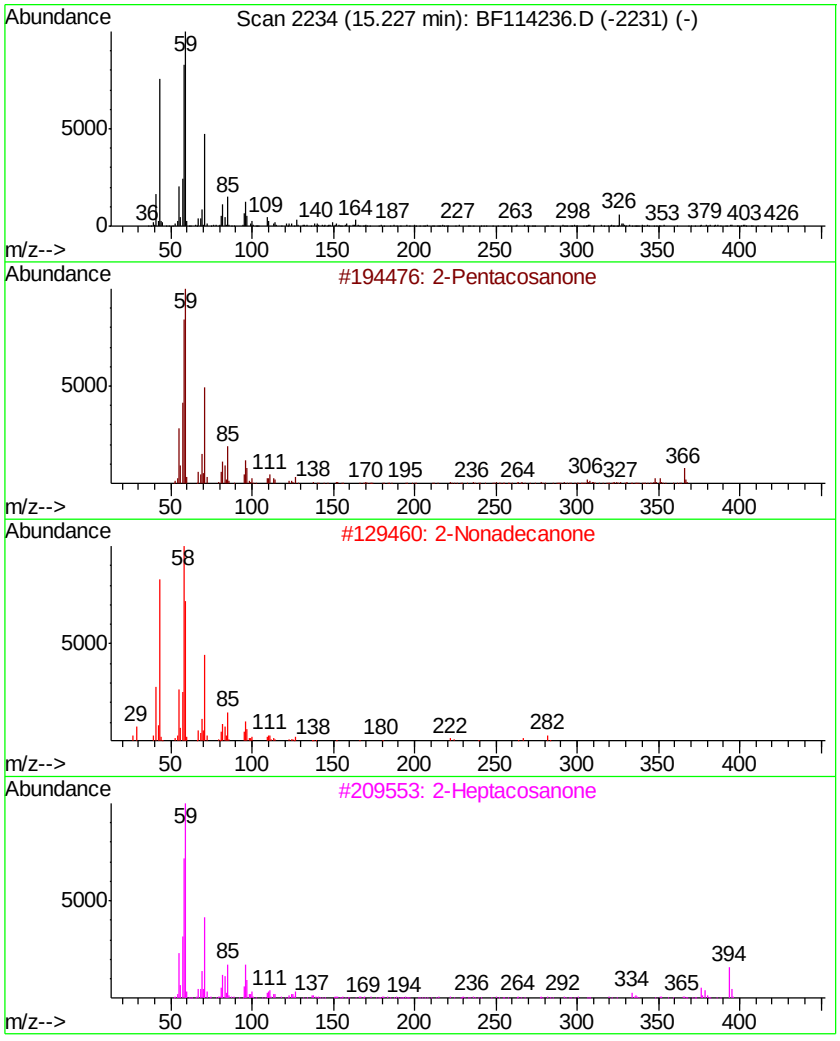
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

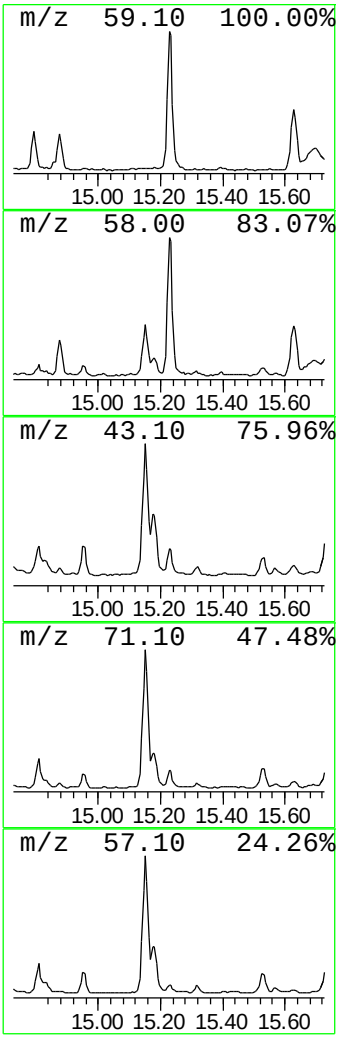
****

Peak Number 12 2-Pentacosanone Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	13.14 ng	1280990	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentacosanone	366	C25H50O	075207-54-4	78
2	2-Nonadecanone	282	C19H38O	000629-66-3	64
3	2-Heptacosanone	394	C27H54O	007796-19-2	58
4	2-Hexadecanone	240	C16H32O	018787-63-8	50
5	2-Heptadecanone	254	C17H34O	002922-51-2	47





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

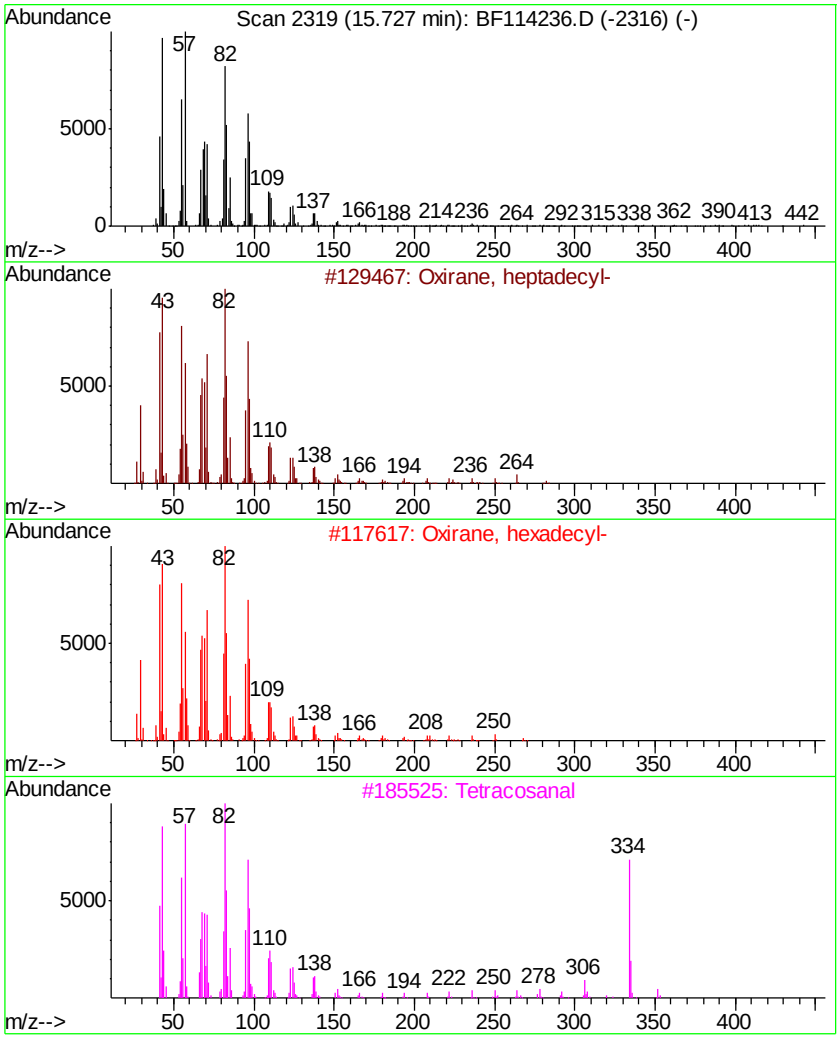
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

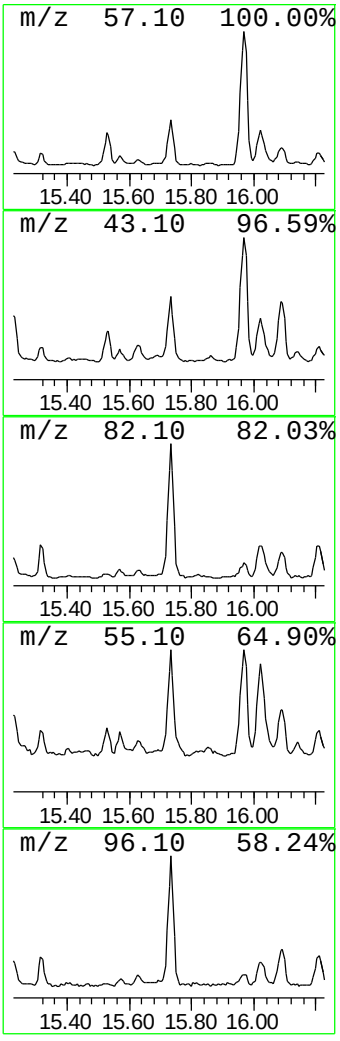
****

Peak Number 13 Oxirane, heptadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	20.44 ng	1993220	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Tetracosanal	352	C24H48O	057866-08-7	91
4	17-Octadecenal	266	C18H34O	056554-86-0	91
5	Octadecanal	268	C18H36O	000638-66-4	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

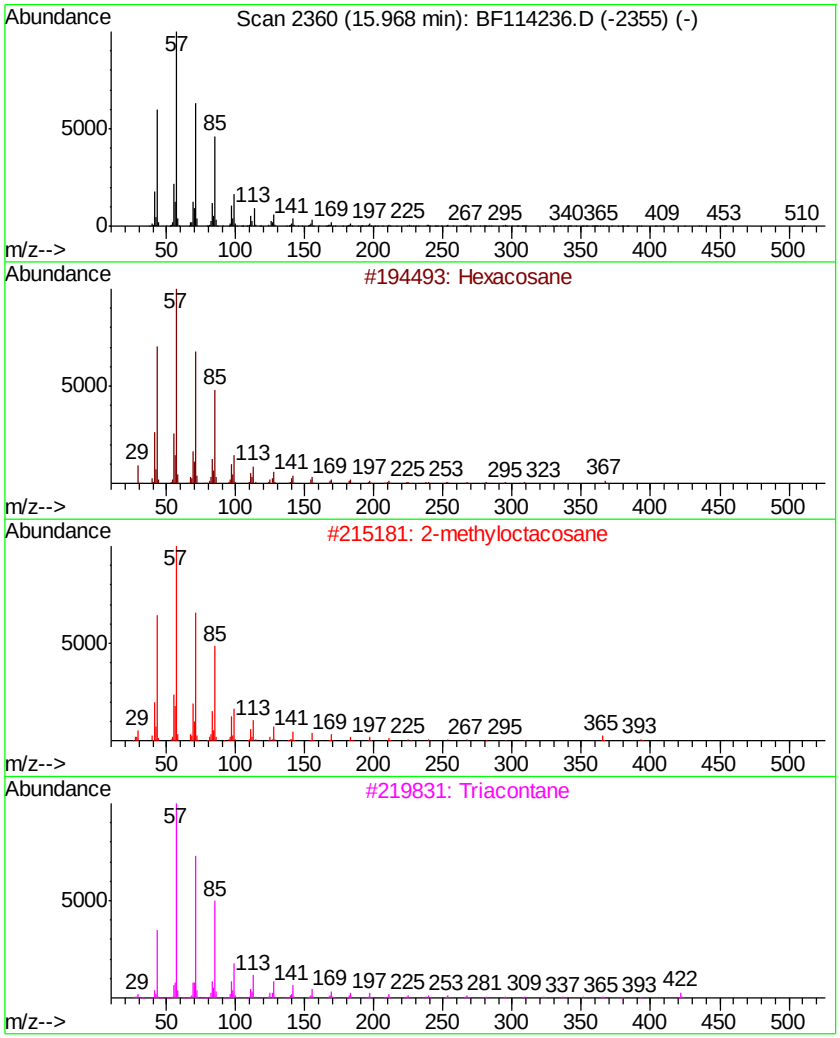
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

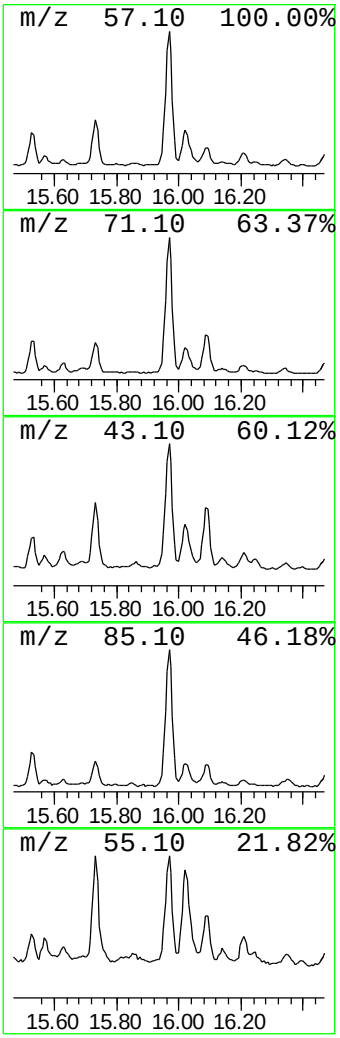
****

Peak Number 14 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	26.82 ng	2615170	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heptacosane	380	C27H56	000593-49-7	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

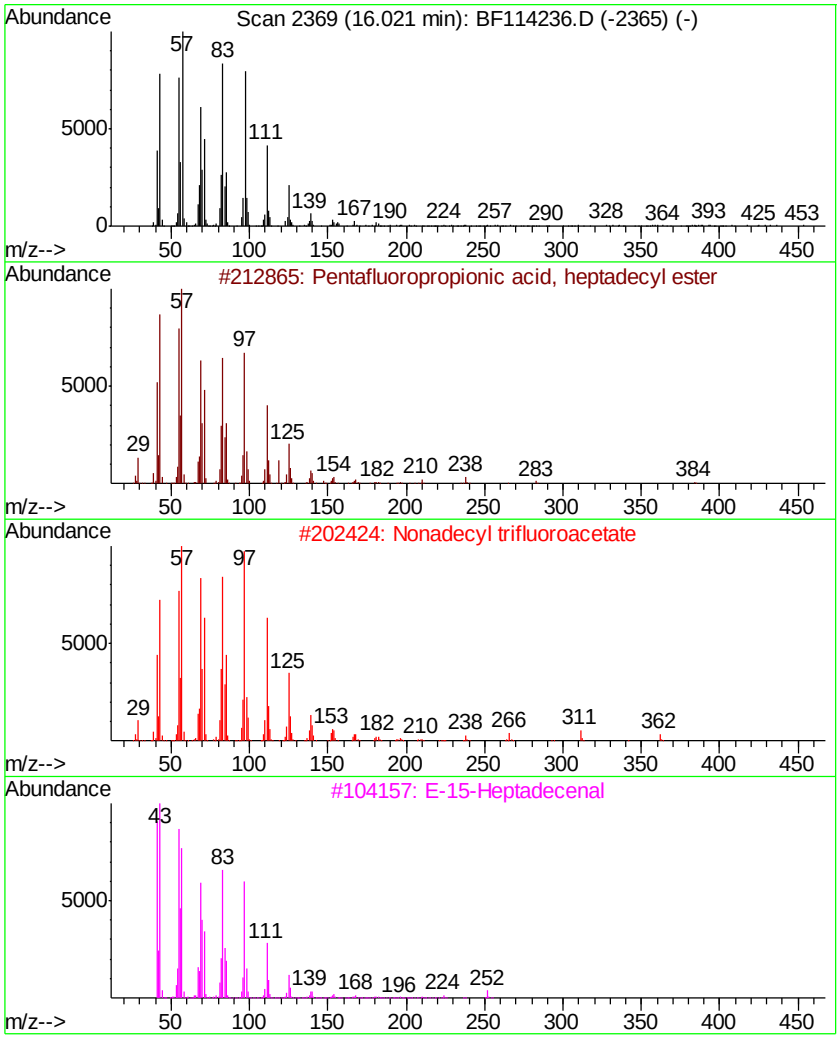
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

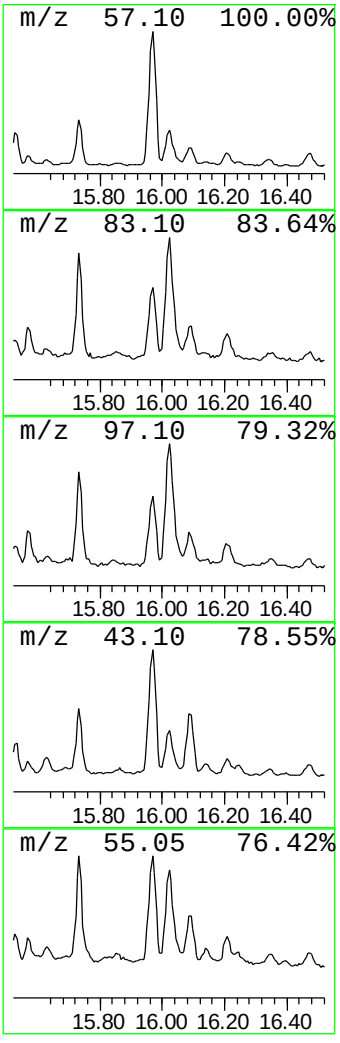
****

Peak Number 15 Pentafluoropropionic acid, ... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	13.28 ng	1295380	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
2	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	87
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
5	1-Heneicosanol	312	C21H44O	015594-90-8	76





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

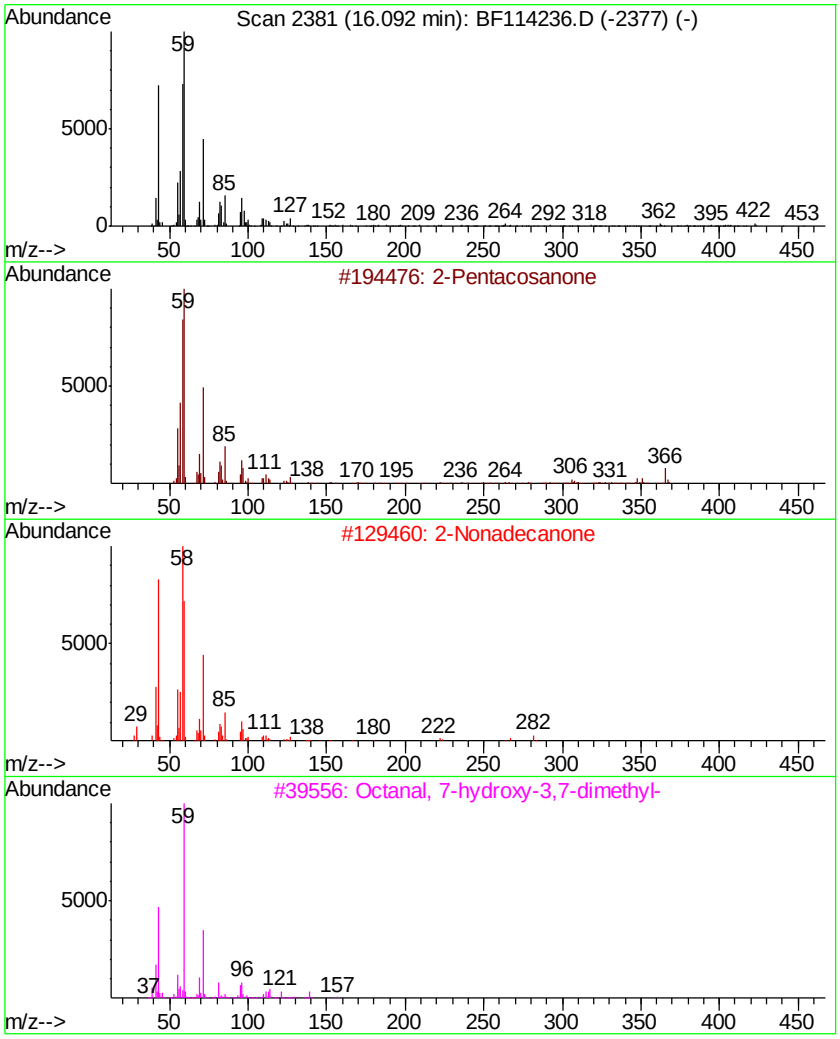
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

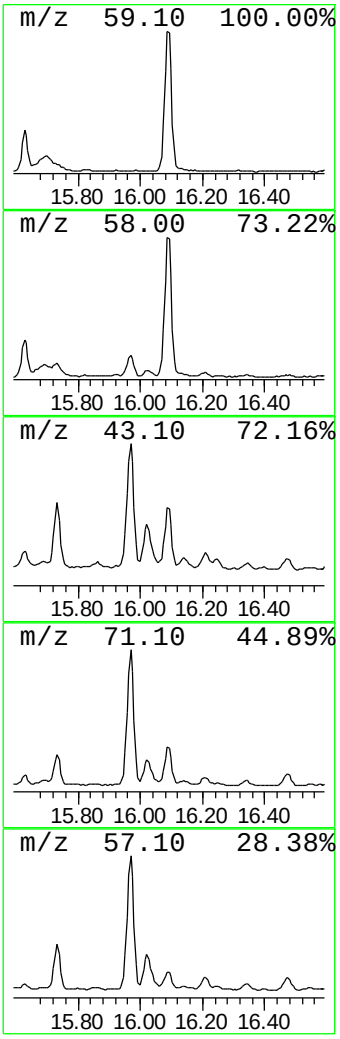
****

Peak Number 16 2-Nonadecanone Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	11.61 ng	1132100	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentacosanone	366	C25H50O	075207-54-4	78
2	2-Nonadecanone	282	C19H38O	000629-66-3	59
3	Octanal, 7-hydroxy-3,7-dimethyl-	172	C10H20O2	000107-75-5	50
4	Oxirane, 3-ethyl-2,2-dimethyl-	100	C6H12O	001192-22-9	50
5	2-Pentadecanone	226	C15H30O	002345-28-0	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

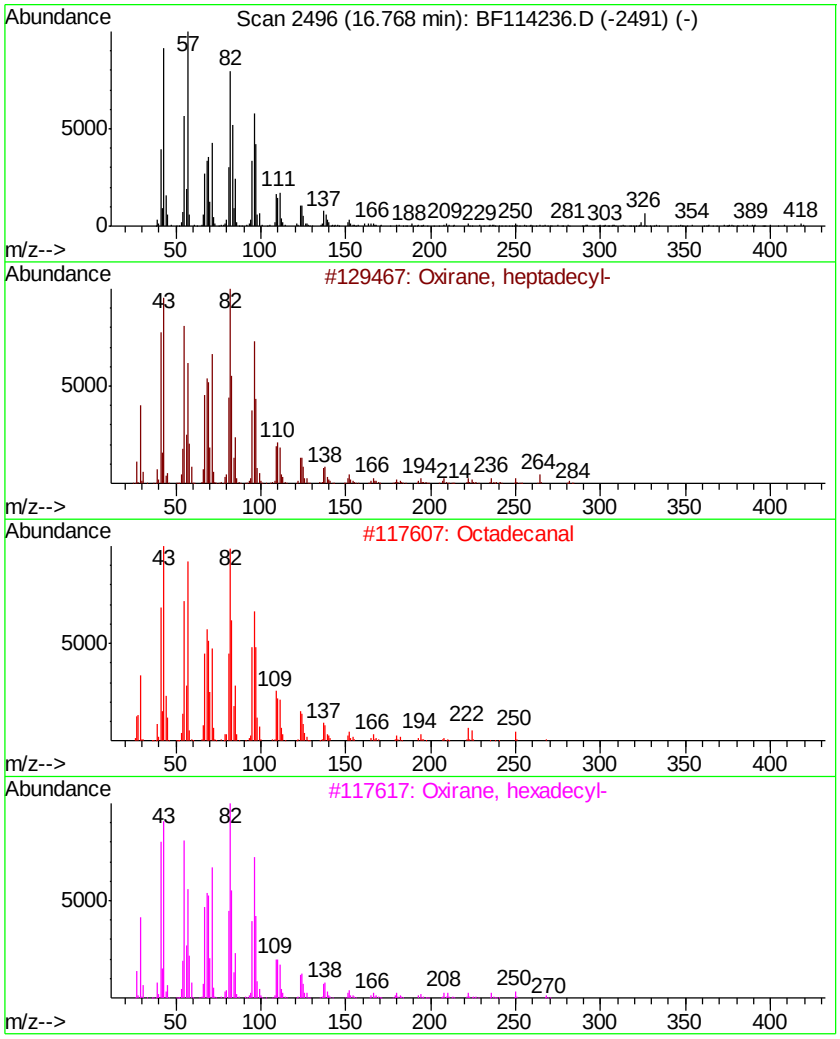
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

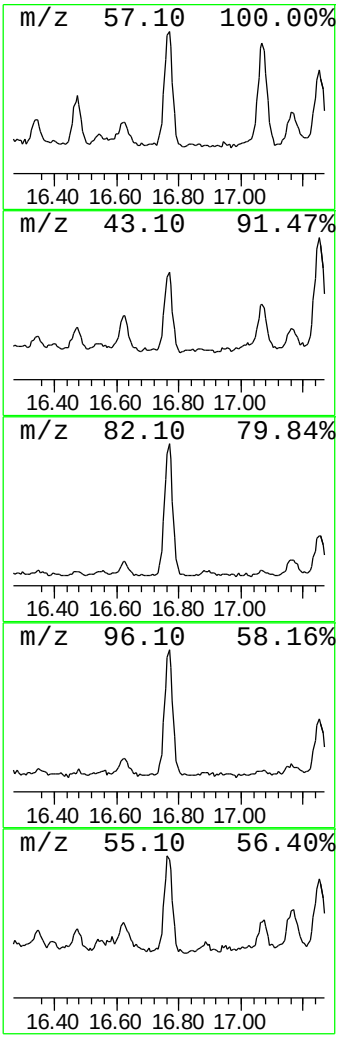
****

Peak Number 17 14-Octadecenal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	16.19 ng	1578900	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
2	Octadecanal	268	C18H36O	000638-66-4	87
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
4	14-Octadecenal	266	C18H34O	056554-89-3	58
5	Undecane, 5-cyclohexyl-	238	C17H34	013151-80-9	49





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

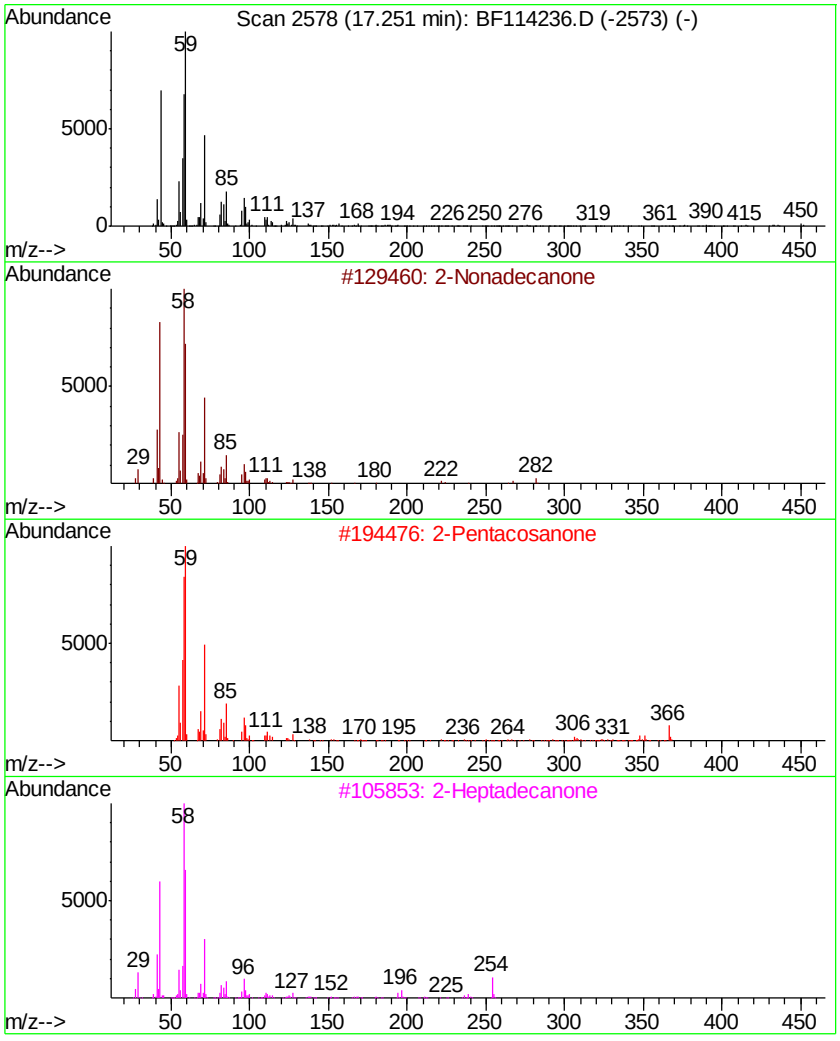
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

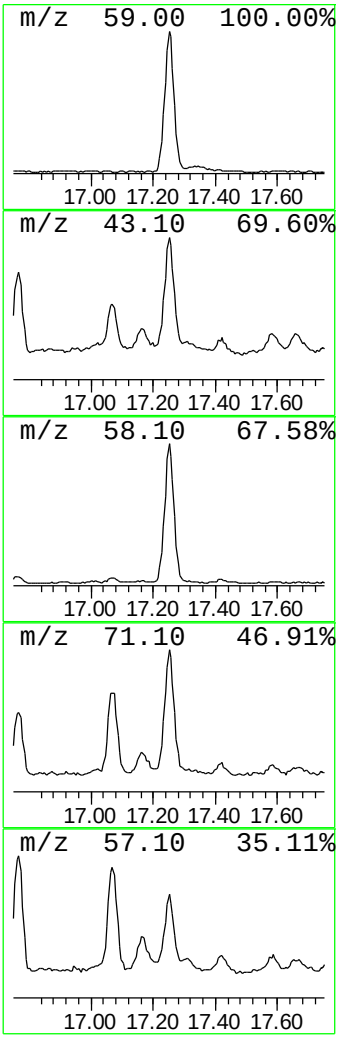
****

Peak Number 18 2-Heptadecanone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.25	15.17 ng	1479030	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonadecanone	282	C19H38O	000629-66-3	93
2	2-Pentacosanone	366	C25H50O	075207-54-4	91
3	2-Heptadecanone	254	C17H34O	002922-51-2	59
4	Oxirane, 3-ethyl-2,2-dimethyl-	100	C6H12O	001192-22-9	50
5	2-Pentadecanone	226	C15H30O	002345-28-0	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

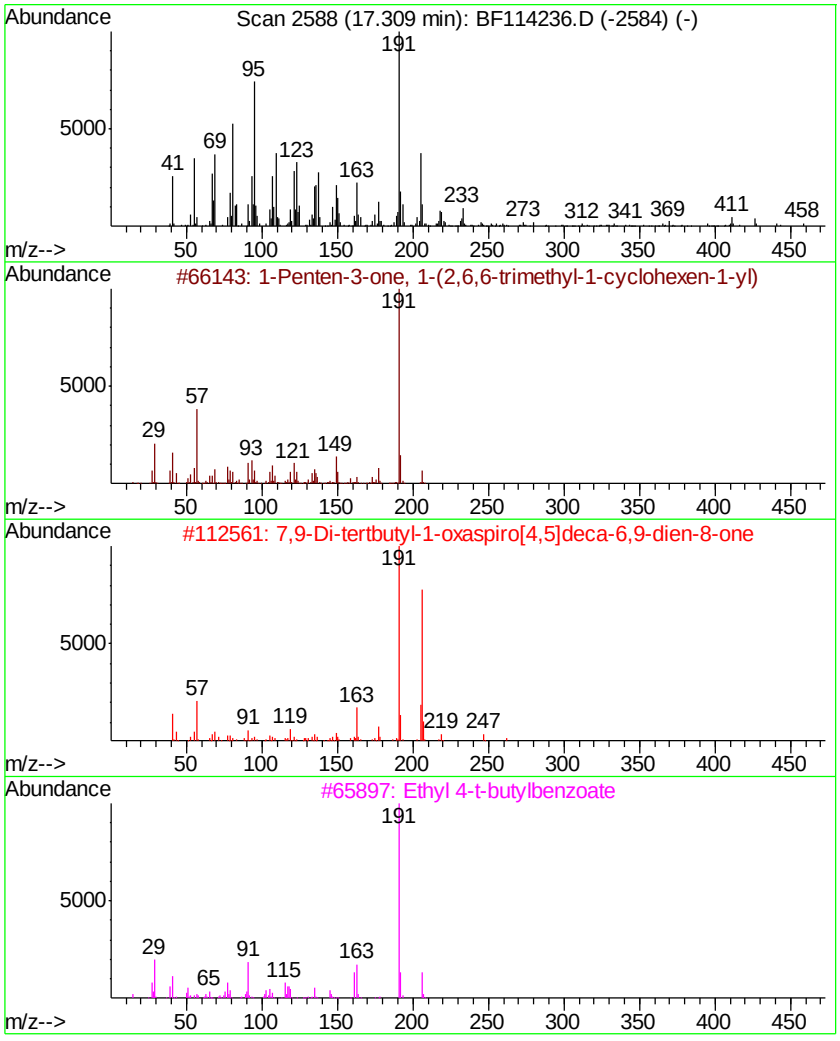
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

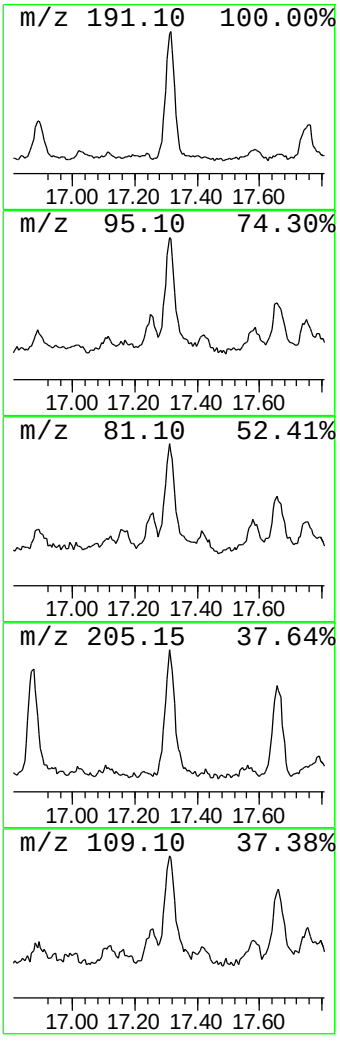
****

Peak Number 19 unknown17.31 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.31	14.41 ng	1405340	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
2	7,9-Di-tertbutyl-1-oxaspiro[4,5]...	262	C17H26O2	138345-00-3	35
3	Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	35
4	5-Fluoro-2-trifluoromethylbenzoi...	290	C14H14F4O2	1000357-62-6	27
5	2-Amino-4-methyl-6-(2-thienyl)py...	191	C9H9N3S	026963-43-9	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

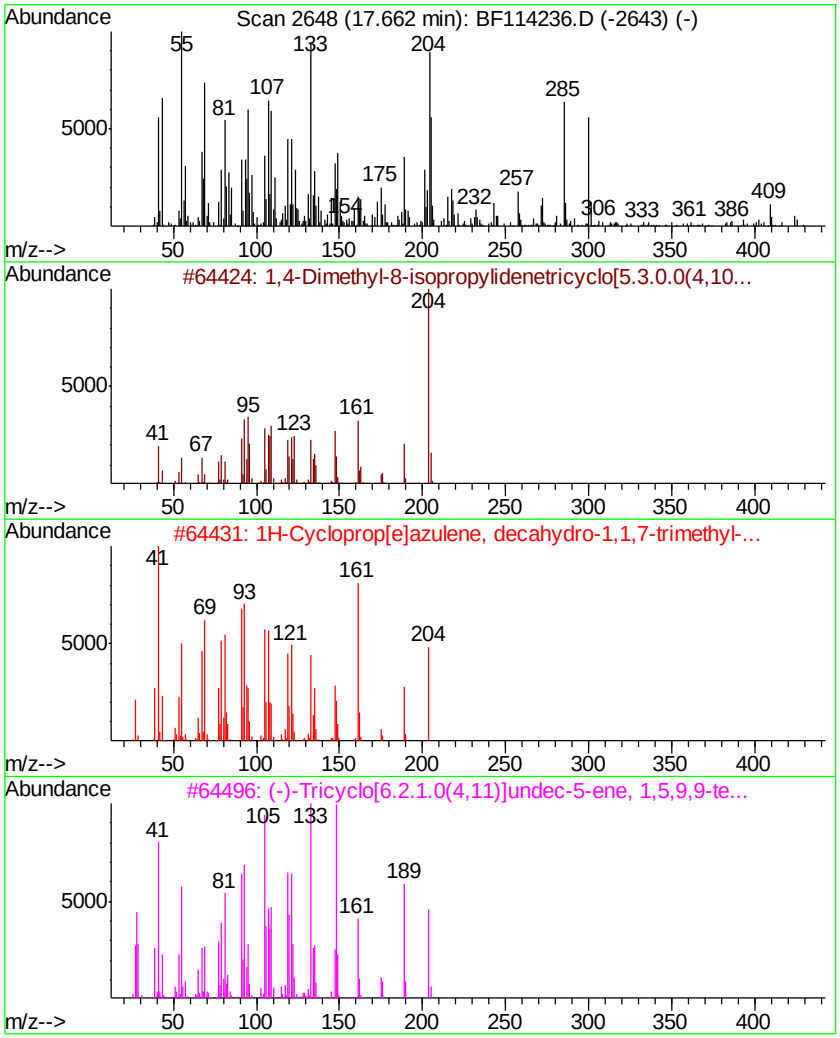
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

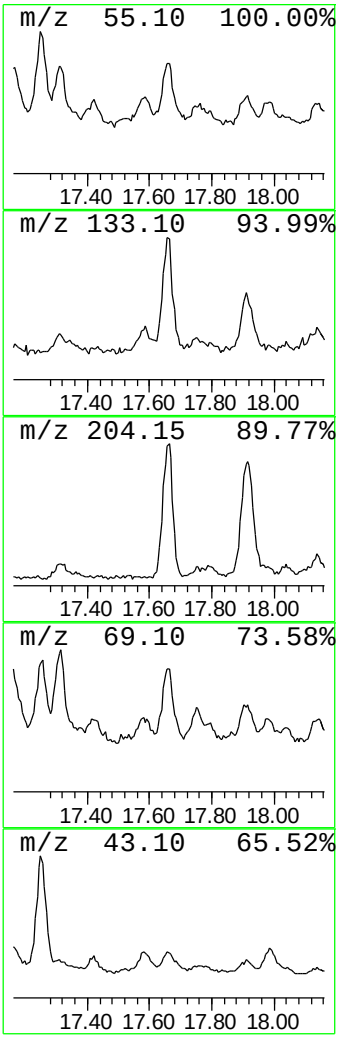
****

Peak Number 20 1,4-Dimethyl-8-isopropylide... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.66	14.80 ng	1442780	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	56
2	1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	51
3	(-)-Tricyclo[6.2.1.0(4,11)]undec...	204	C15H24	1000154-06-7	46
4	Humulane-1,6-dien-3-ol	222	C15H26O	1000140-23-1	38
5	D-Friedoolean-14-en-3-one	424	C30H48O	000514-07-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051319\
Data File : BF114236.D
Acq On : 13 May 2019 18:26
Operator : JU/SJ
Sample : K2768-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P026-SS014-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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
Butane, 2-methoxy...	2.13	23.7	ng	1933020	1	6.86	1633300	20.0
unknown6.64	6.64	82.7	ng	6751350	1	6.86	1633300	20.0
n-Hexadecanoic acid	11.90	14.0	ng	1564730	4	11.38	2231490	20.0
Docosane	13.53	10.0	ng	837645	5	14.03	1680250	20.0
Caparratriene	13.78	65.3	ng	5489590	5	14.03	1680250	20.0
Ethanol, 2-(tetra...	13.86	160.5	ng	13484900	5	14.03	1680250	20.0
Eicosane	14.50	101.3	ng	8513110	5	14.03	1680250	20.0
Octadecanal	14.95	11.5	ng	1120280	6	15.52	1950260	20.0
Heptadecane, 9-oc...	15.15	42.4	ng	4129710	6	15.52	1950260	20.0
1-Heneicosanol	15.18	24.8	ng	2415230	6	15.52	1950260	20.0
2-Pentacosanone	15.23	13.1	ng	1280990	6	15.52	1950260	20.0
Oxirane, heptadecyl-	15.73	20.4	ng	1993220	6	15.52	1950260	20.0
Hexacosane	15.97	26.8	ng	2615170	6	15.52	1950260	20.0
Pentafluoropropio...	16.02	13.3	ng	1295380	6	15.52	1950260	20.0
2-Nonadecanone	16.09	11.6	ng	1132100	6	15.52	1950260	20.0
14-Octadecenal	16.77	16.2	ng	1578900	6	15.52	1950260	20.0
2-Heptadecanone	17.25	15.2	ng	1479030	6	15.52	1950260	20.0
unknown17.31	17.31	14.4	ng	1405340	6	15.52	1950260	20.0
1,4-Dimethyl-8-is...	17.66	14.8	ng	1442780	6	15.52	1950260	20.0