LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118404.D
Acq On : 31 Dec 2019 14:40
Operator : JU
Sample : K6465-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

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-BF122419.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	5.057	501	505	521	rVB	196384	235445	11.66%	1.117%
2	5.475	572	576	598	rBV	1293676	1395609	69.14%	6.620%
3	6.487	744	748	765	rBV	1451882	1588932	78.72%	7.537%
4	6.622	767	771	778	rVV	1896862	1686571	83.55%	8.000%
5	6.851	807	810	818	rBV	616017	479496	23.75%	2.274%
6	7.010	833	837	850	rBV	1321593	1240394	61.45%	5.883%
7	7.416	902	906	922	rBV	972320	950605	47.09%	4.509%
8	8.139	1025	1029	1048	rBV	628743	667222	33.05%	3.165%
9	9.216	1208	1212	1224	rBV	1932792	1738200	86.11%	8.245%
10	9.616	1276	1280	1287	rVB	127988	139660	6.92%	0.662%
11	9.898	1324	1328	1333	rBV	845800	813841	40.32%	3.860%
12	9.933	1333	1334	1342	rVB	42483	30309	1.50%	0.144%
13	10.110	1360	1364	1369	rBV	18266	22379	1.11%	0.106%
14	10.451	1419	1422	1427	rBV	30705	32725	1.62%	0.155%
15	10.698	1460	1464	1476	rBV	1438046	1454614	72.06%	6.900%
16	11.004	1508	1516	1519	rBV4	13672	23099	1.14%	0.110%
17	11.392	1579	1582	1585	rBV	926019	934470	46.29%	4.432%
18	11.421	1585	1587	1591	rVV	258230	228601	11.32%	1.084%
19	11.474	1591	1596	1599	rVV	59934	72249	3.58%	0.343%
20	11.633	1617	1623	1627	rBV4	26857	52016	2.58%	0.247%
21	11.916	1665	1671	1679	rBV4	140351	257602	12.76%	1.222%
22	11.974	1679	1681	1684	rBV	27211	25601	1.27%	0.121%
23	12.010	1684	1687	1690	rBV	75684	87899	4.35%	0.417%
24	12.192	1716	1718	1721	rBV	28953	22353	1.11%	0.106%
25	12.451	1759	1762	1765	rBV	46599	48589	2.41%	0.230%
26	12.616	1787	1790	1795	rBV	317062	262057	12.98%	1.243%
27	12.704	1803	1805	1813	rVB5	27721	36342	1.80%	0.172%
28	12.845	1823	1829	1836	rBV	325193	360004	17.83%	1.708%
29	12.986	1848	1853	1856	rBV	2315693	2018552	100.00%	9.574%
30	13.068	1862	1867	1873	rVB6	28642	53913	2.67%	0.256%
31	13.174	1882	1885	1888	rVB	55274	52301	2.59%	0.248%
32	13.204	1888	1890	1893	rVB	66379	53835	2.67%	0.255%
33	13.245	1894	1897	1900	rBV	54802	47018	2.33%	0.223%
34	13.280	1900	1903	1911	rVB3	41187	62174	3.08%	0.295%

LSC Area Percent Report

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Acq On : 31 Dec 2019 14:40
Operator : JU
Sample : K6465-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

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-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.374	1916	1919	1922	rVB2	25504	24473	1.21%	0.116%
36	13.410	1922	1925	1931	rBV2	23630	30482	1.51%	0.145%
37	13.551	1944	1949	1951	rBV	83914	80844	4.01%	0.383%
38	13.804	1988	1992	1994	rBV	32138	31333	1.55%	0.149%
39	13.880	2002	2005	2015	rVB2	200960	280106	13.88%	1.329%
40	14.051	2026	2034	2037	rBV2	844442	916532	45.41%	4.347%
41	14.080	2037	2039	2043	rVB	126262	117570	5.82%	0.558%
42	14.198	2055	2059	2061	rBV	92606	86831	4.30%	0.412%
43	14.321	2077	2080	2086	rVB7	27436	32804	1.63%	0.156%
44	14.445	2099	2101	2104	rVB2	28697	25602	1.27%	0.121%
45	14.504	2108	2111	2113	rBV	127368	106867	5.29%	0.507%
46	14.810	2159	2163	2168	rBV	174381	192473	9.54%	0.913%
47	14.957	2185	2188	2193	rBV5	31807	36418	1.80%	0.173%
48	15.109	2211	2214	2217	rBV	53869	74193	3.68%	0.352%
49	15.157	2217	2222	2226	rVB2	200457	252712	12.52%	1.199%
50	15.227	2231	2234	2240	rVB5	19923	30259	1.50%	0.144%
51	15.421	2263	2267	2273	rVV	34464	47025	2.33%	0.223%
52	15.486	2274	2278	2282	rVV	52918	74313	3.68%	0.352%
53	15.545	2282	2288	2301	rVB2	596732	920502	45.60%	4.366%
54	15.980	2357	2362	2371	rBV	159828	266743	13.21%	1.265%
55	16.498	2444	2450	2458	rVB2	91985	165981	8.22%	0.787%
56	17.086	2543	2550	2561	rBV6	39368	114079	5.65%	0.541%

Sum of corrected areas: 21082819

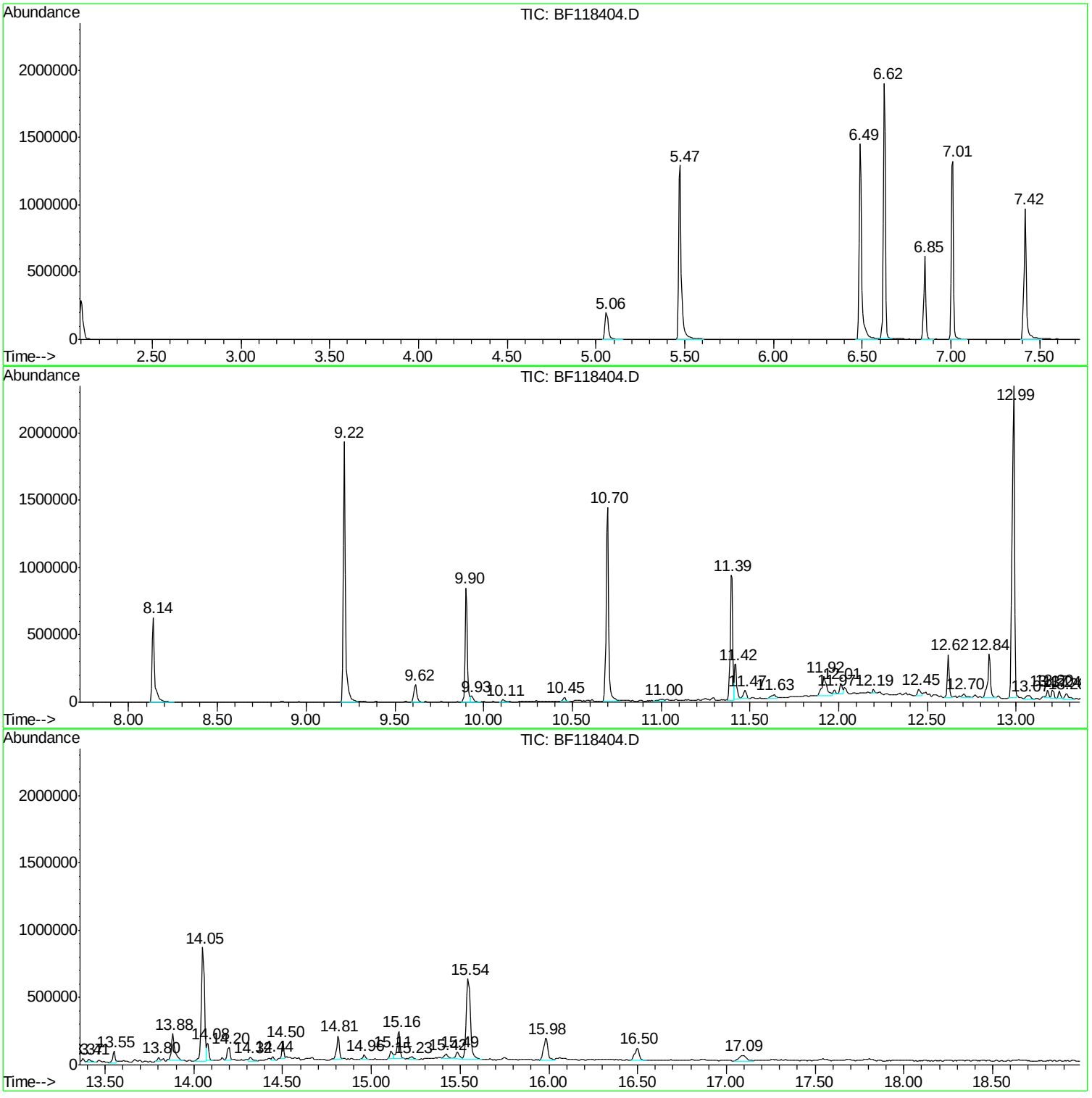
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118404.D
Acq On : 31 Dec 2019 14:40
Operator : JU
Sample : K6465-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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\BF123119\
Data File : BF118404.D
Acq On : 31 Dec 2019 14:40
Operator : JU
Sample : K6465-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

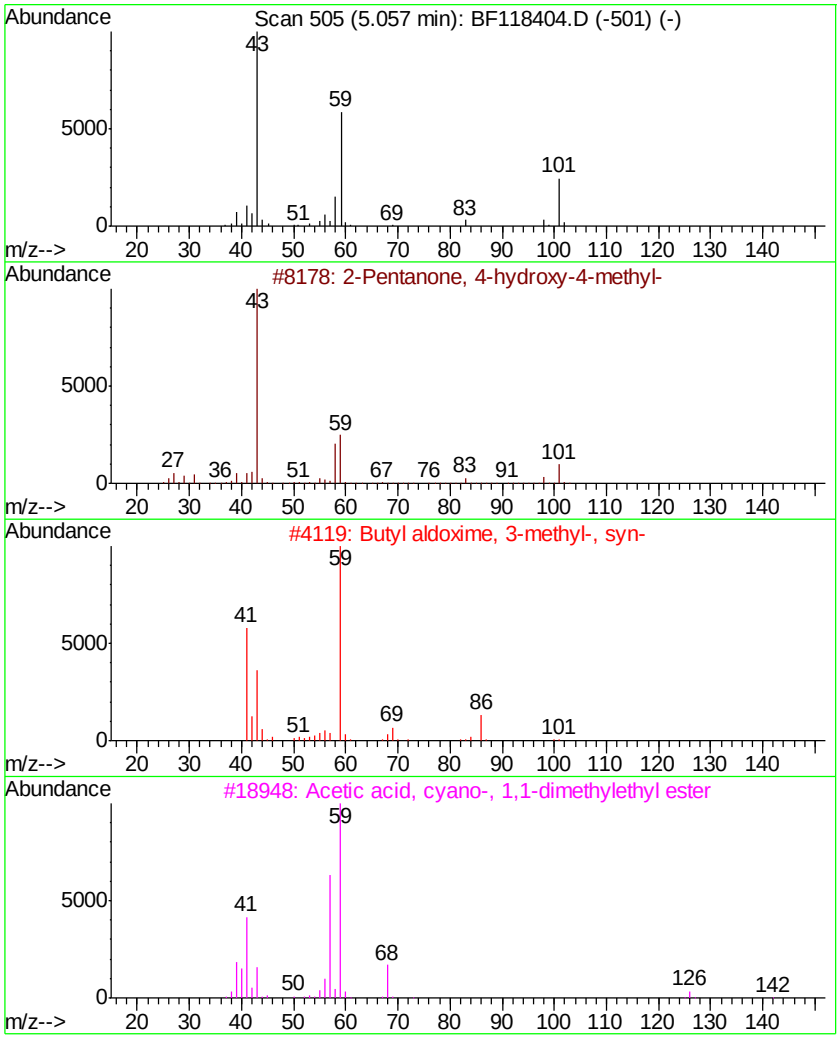
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

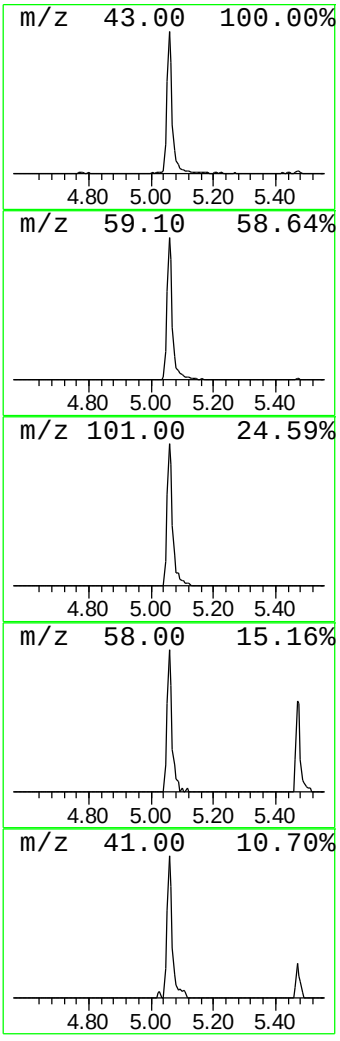
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	9.82 ng	235445	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118404.D
Acq On : 31 Dec 2019 14:40
Operator : JU
Sample : K6465-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

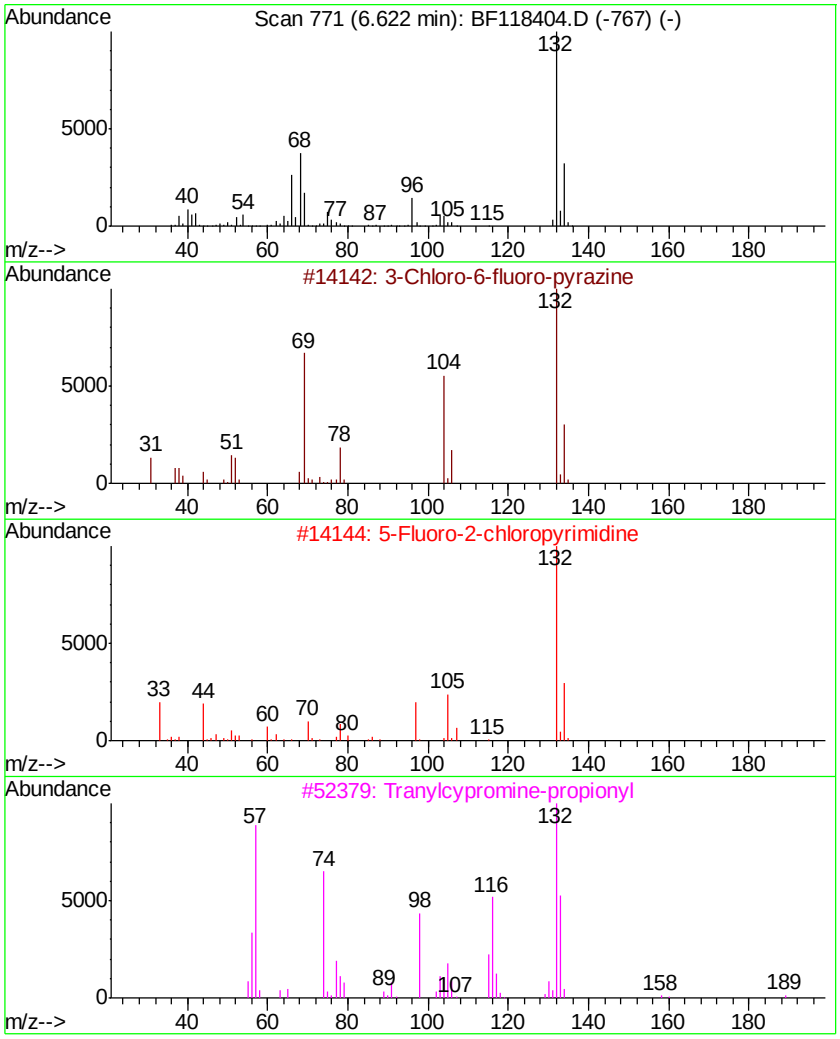
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

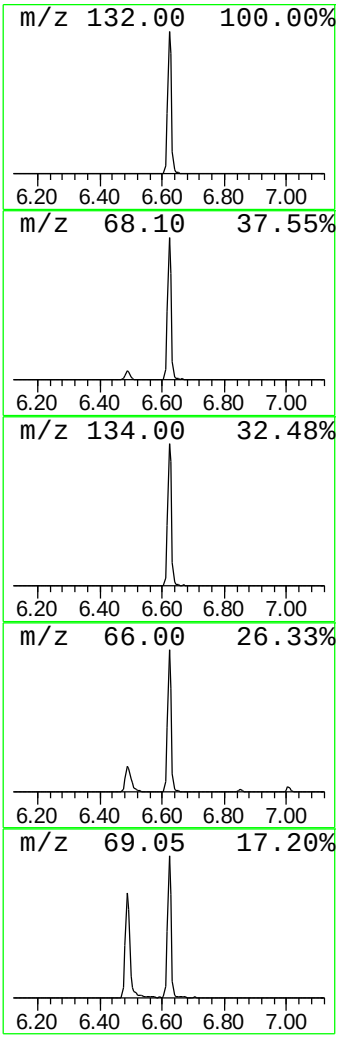
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	70.35 ng	1686570	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118404.D
Acq On : 31 Dec 2019 14:40
Operator : JU
Sample : K6465-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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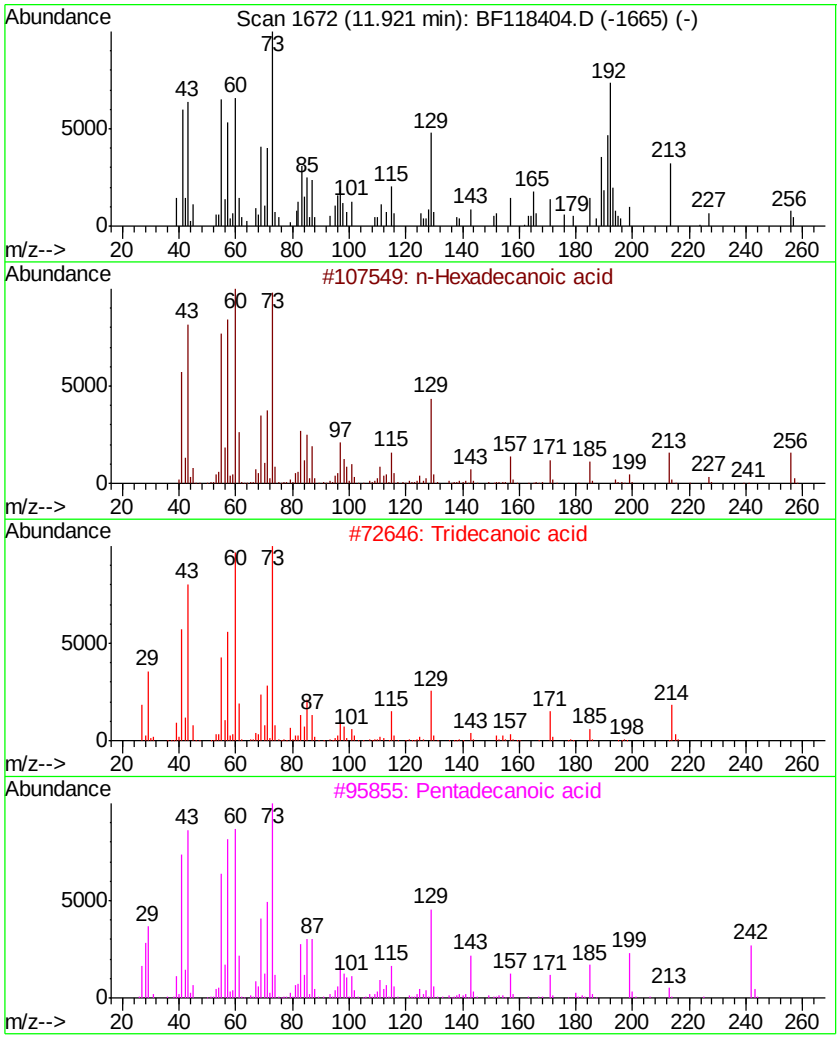
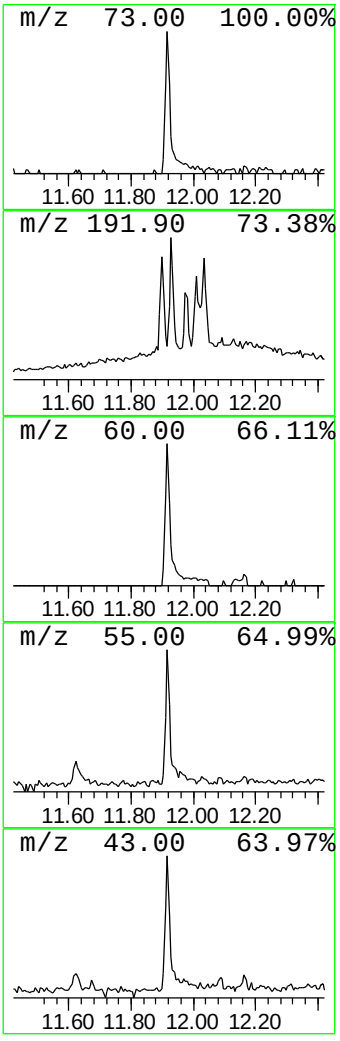
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	5.51 ng	257602	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118404.D
Acq On : 31 Dec 2019 14:40
Operator : JU
Sample : K6465-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

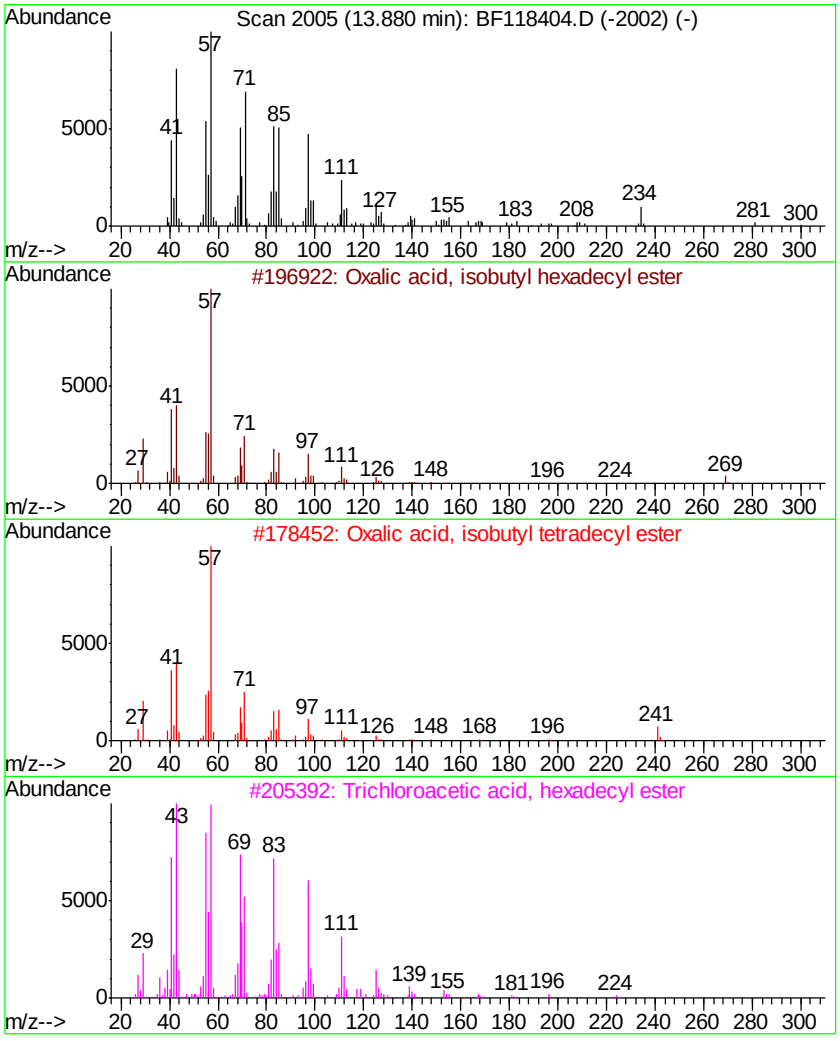
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

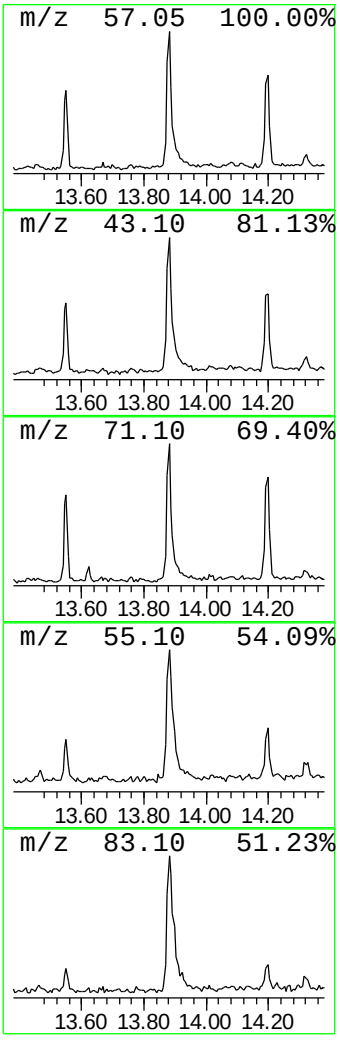
****

Peak Number 5 Oxalic acid, isobutyl hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	6.11 ng	280106	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
5	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	87





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Sample : K6465-04
Misc :
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Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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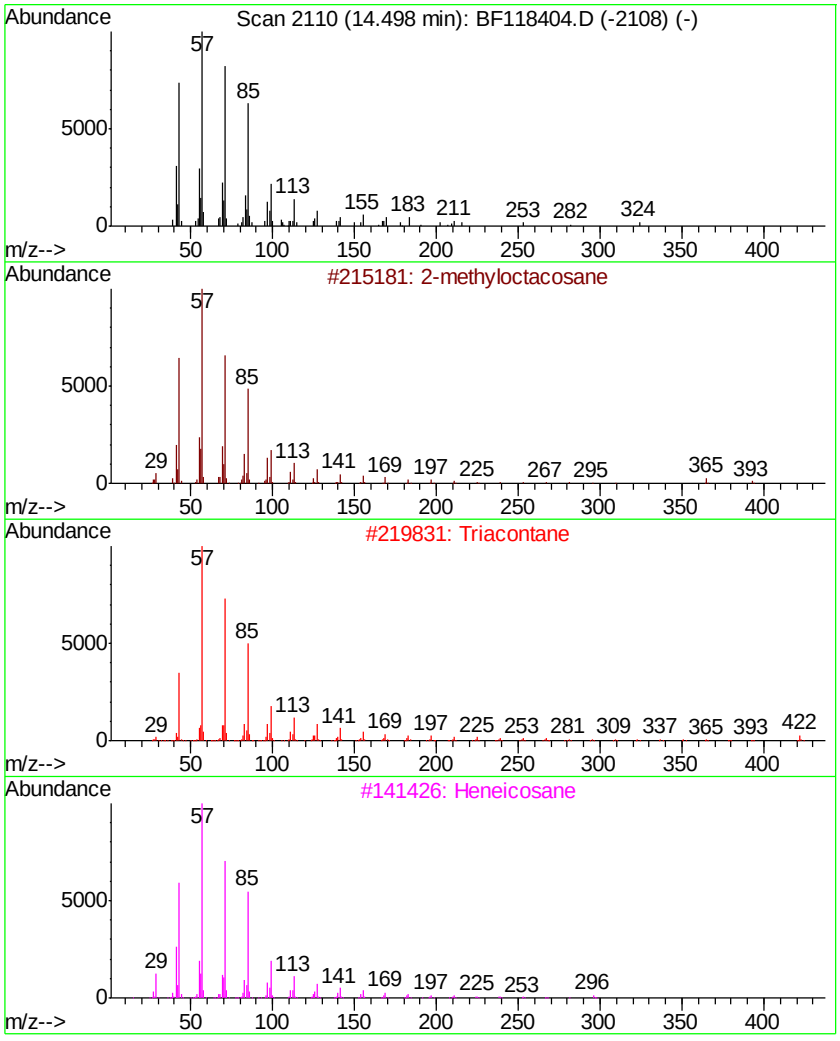
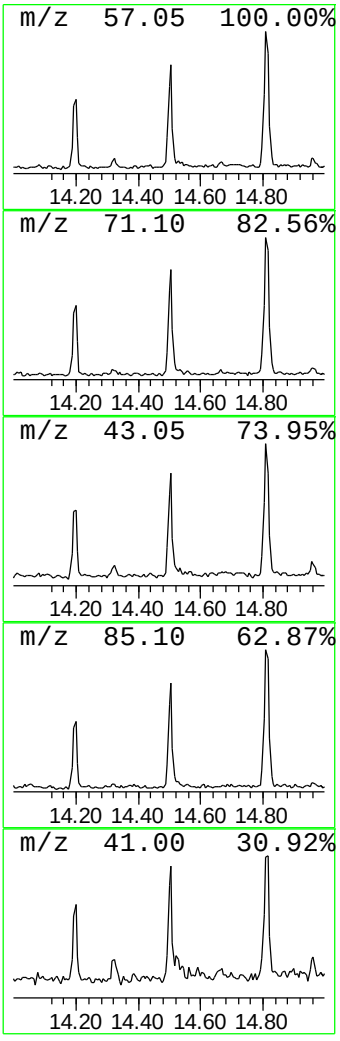
Peak Number 6 2-methyloctacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.33 ng	106867	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Triacontane	422	C30H62	000638-68-6	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Heptadecane	240	C17H36	000629-78-7	90





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Sample : K6465-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

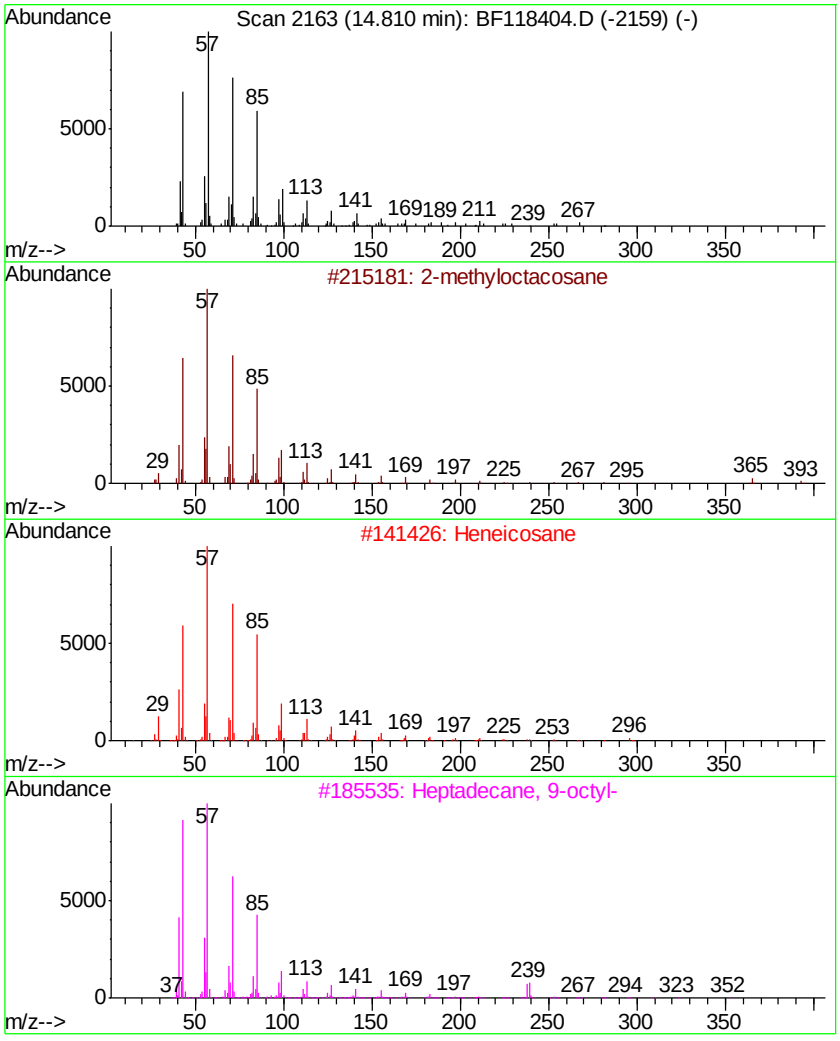
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

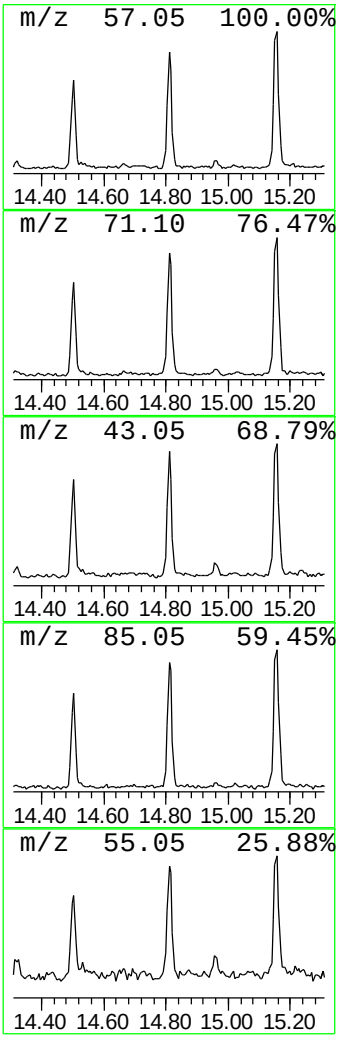
****

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	4.18 ng	192473	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Hexadecane	226	C16H34	000544-76-3	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118404.D
Acq On : 31 Dec 2019 14:40
Operator : JU
Sample : K6465-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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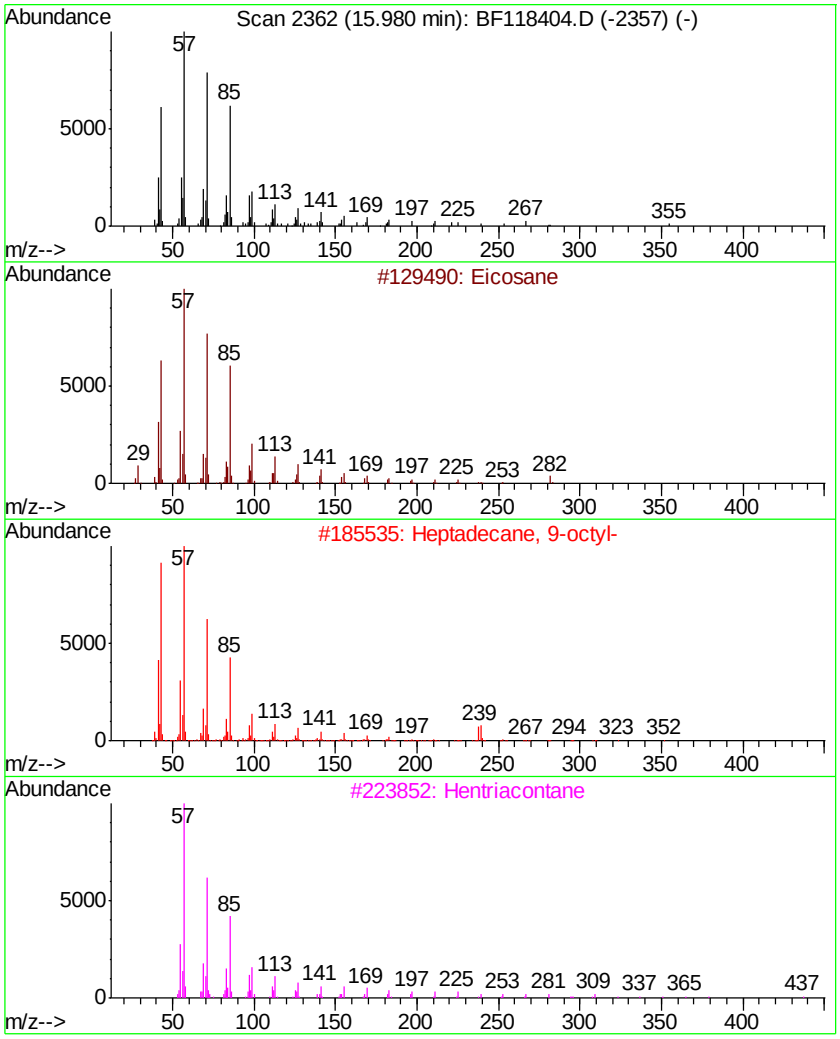
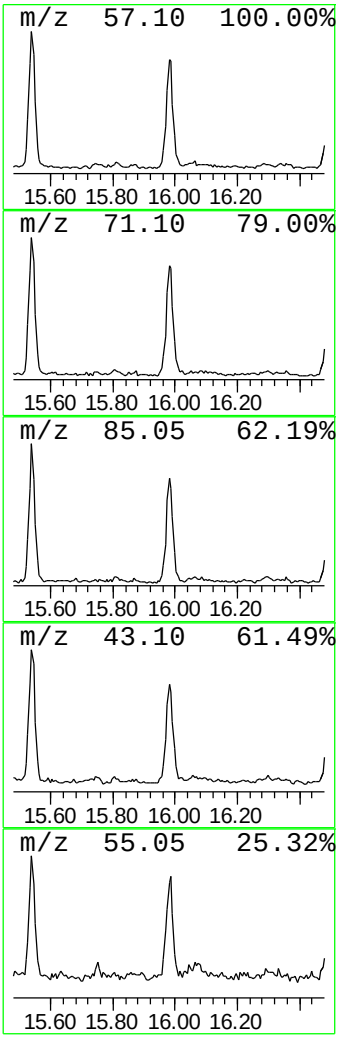
Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	5.80 ng	266743	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Docosane	310	C22H46	000629-97-0	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118404.D
Acq On : 31 Dec 2019 14:40
Operator : JU
Sample : K6465-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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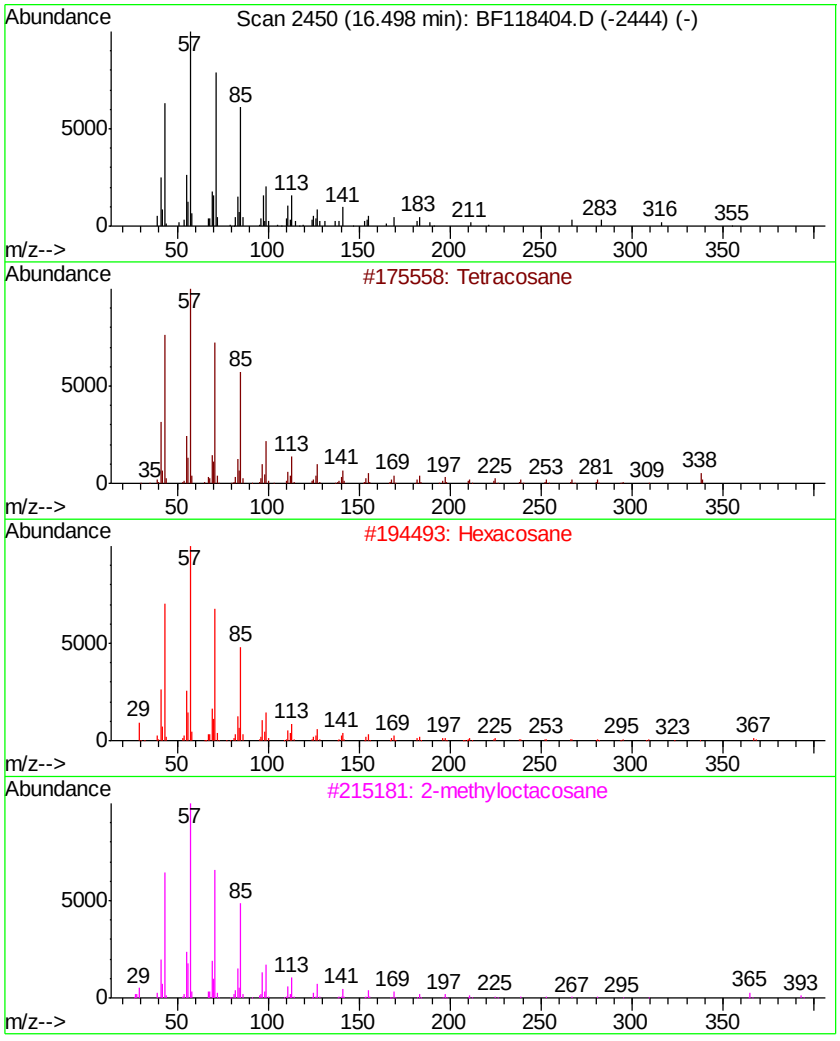
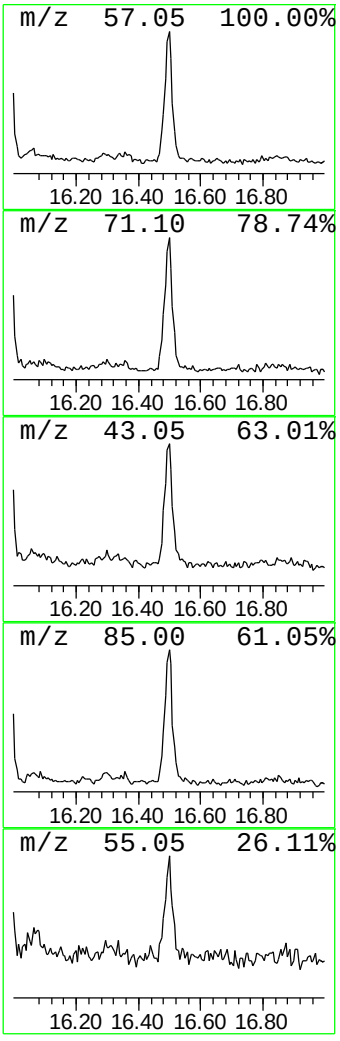
Peak Number 9 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	3.61 ng	165981	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF123119\
Data File : BF118404.D
Acq On : 31 Dec 2019 14:40
Operator : JU
Sample : K6465-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-10-(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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
2-Pentanone, 4-hy...	5.06	9.8	ng	235445	1	6.85	479496	20.0
unknown6.62	6.62	70.3	ng	1686570	1	6.85	479496	20.0
n-Hexadecanoic acid	11.92	5.5	ng	257602	4	11.40	934470	20.0
Oxalic acid, isob...	13.88	6.1	ng	280106	5	14.05	916532	20.0
2-methyloctacosane	14.50	2.3	ng	106867	5	14.05	916532	20.0
Heptadecane, 9-oc...	14.81	4.2	ng	192473	6	15.55	920502	20.0
Eicosane	15.98	5.8	ng	266743	6	15.55	920502	20.0
Tetracosane	16.50	3.6	ng	165981	6	15.55	920502	20.0