

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF123019\
 Data File : BF118389.D
 Acq On : 30 Dec 2019 19:05
 Operator : JU
 Sample : K6442-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 K615-WC-1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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	523	rVB	330382	416412	12.12%	1.419%
2	5.469	571	575	597	rBV	2182375	2221580	64.66%	7.571%
3	6.486	744	748	767	rBV	2232024	2392547	69.64%	8.153%
4	6.622	767	771	775	rBV	2934951	2567640	74.74%	8.750%
5	6.851	807	810	816	rBV	885796	708685	20.63%	2.415%
6	7.010	833	837	840	rBV	2329074	2012160	58.57%	6.857%
7	7.416	902	906	918	rBV	1508632	1492522	43.44%	5.086%
8	8.139	1025	1029	1049	rVB	926921	930774	27.09%	3.172%
9	9.216	1208	1212	1223	rBV	3761244	3264756	95.03%	11.125%
10	9.616	1276	1280	1289	rVB	166986	187148	5.45%	0.638%
11	9.898	1320	1328	1340	rVB	1242016	1161496	33.81%	3.958%
12	10.692	1459	1463	1479	rBV	2134759	2249224	65.47%	7.665%
13	11.392	1578	1582	1585	rBV	1256854	1178933	34.32%	4.018%
14	11.416	1585	1586	1591	rVB	214278	161216	4.69%	0.549%
15	11.621	1616	1621	1628	rBV4	45714	91197	2.65%	0.311%
16	11.916	1665	1671	1679	rBV2	420566	492248	14.33%	1.677%
17	12.615	1786	1790	1795	rBV	264606	266238	7.75%	0.907%
18	12.704	1802	1805	1812	rBV3	97666	121151	3.53%	0.413%
19	12.845	1823	1829	1835	rBV	236155	246882	7.19%	0.841%
20	12.986	1848	1853	1856	rBV	3942137	3435536	100.00%	11.707%
21	13.174	1878	1885	1887	rBV4	29372	64671	1.88%	0.220%
22	13.804	1988	1992	1993	rBV2	34119	40866	1.19%	0.139%
23	13.880	2001	2005	2015	rVB2	338680	549291	15.99%	1.872%
24	14.051	2029	2034	2037	rBV	924026	1008965	29.37%	3.438%
25	14.074	2037	2038	2047	rVB2	104768	103371	3.01%	0.352%
26	14.192	2056	2058	2061	rBV	39471	43300	1.26%	0.148%
27	14.498	2108	2110	2113	rBV	77870	86700	2.52%	0.295%
28	14.809	2158	2163	2166	rBV2	68233	88976	2.59%	0.303%
29	15.104	2210	2213	2216	rBV	75186	100411	2.92%	0.342%
30	15.151	2219	2221	2224	rVB	79143	75122	2.19%	0.256%
31	15.409	2262	2265	2270	rBV	76326	94583	2.75%	0.322%
32	15.474	2273	2276	2281	rVV	87555	116177	3.38%	0.396%
33	15.539	2282	2287	2296	rVB2	728356	989150	28.79%	3.371%
34	15.980	2358	2362	2369	rVB3	62371	100219	2.92%	0.342%

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF123019\
Data File : BF118389.D
Acq On : 30 Dec 2019 19:05
Operator : JU
Sample : K6442-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K615-WC-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-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.051	2370	2374	2386	rVB3	52389	148446	4.32%	0.506%
36	16.498	2445	2450	2453	rBV3	32376	56638	1.65%	0.193%
37	17.050	2540	2544	2549	rBV2	44853	79642	2.32%	0.271%

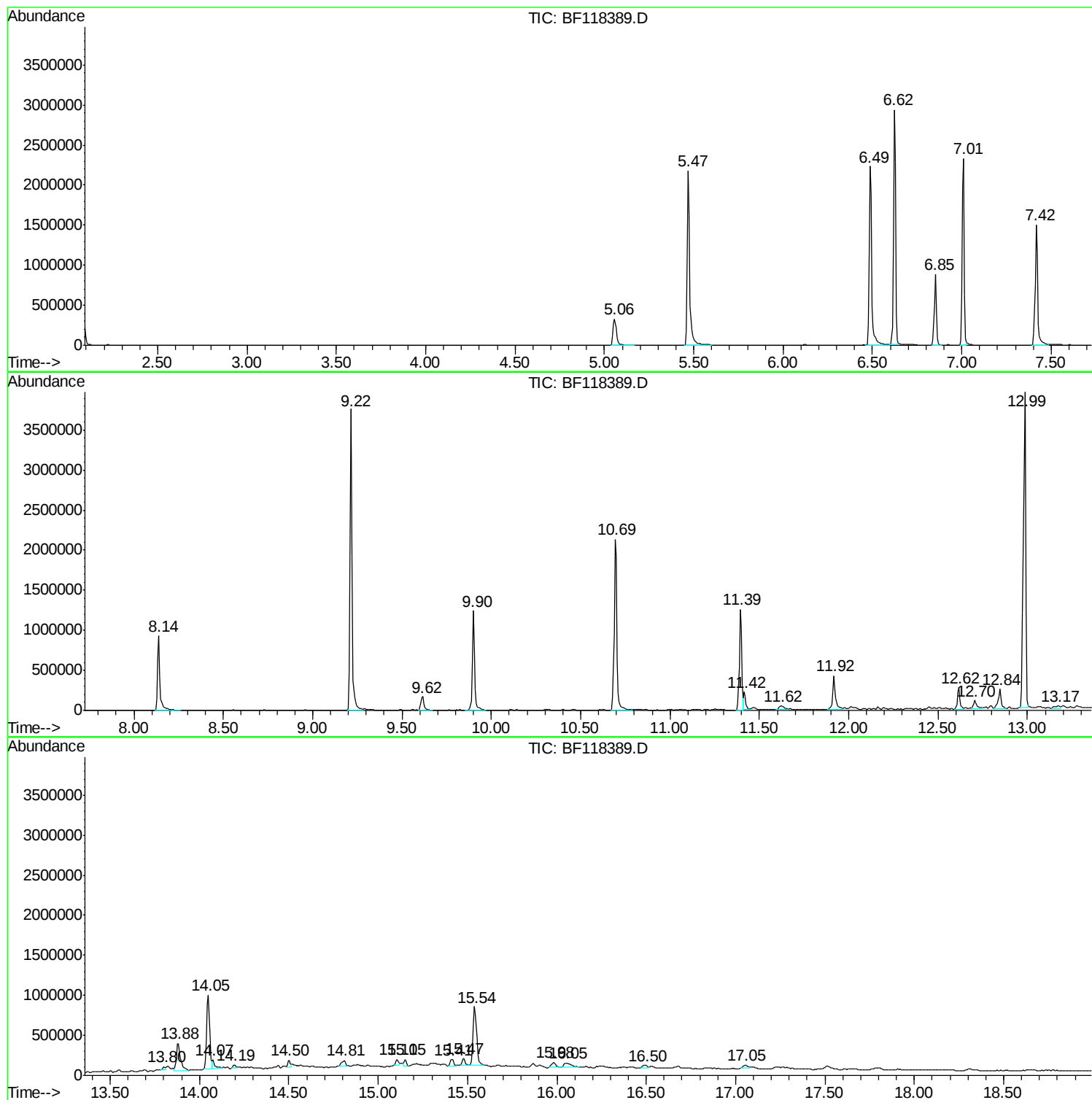
Sum of corrected areas: 29344873

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118389.D
Acq On : 30 Dec 2019 19:05
Operator : JU
Sample : K6442-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K615-WC-1

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\BF123019\
Data File : BF118389.D
Acq On : 30 Dec 2019 19:05
Operator : JU
Sample : K6442-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K615-WC-1

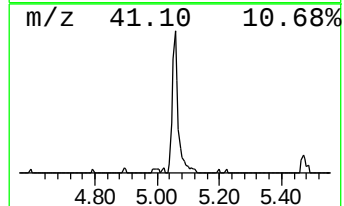
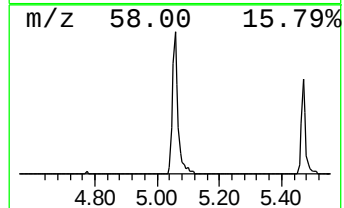
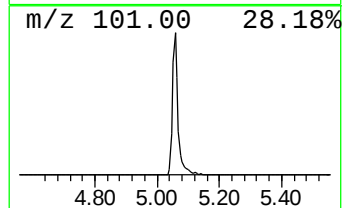
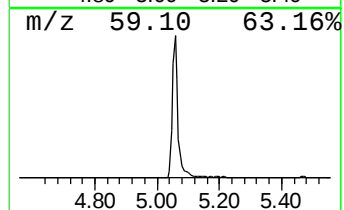
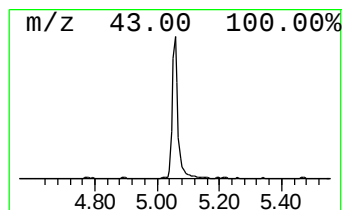
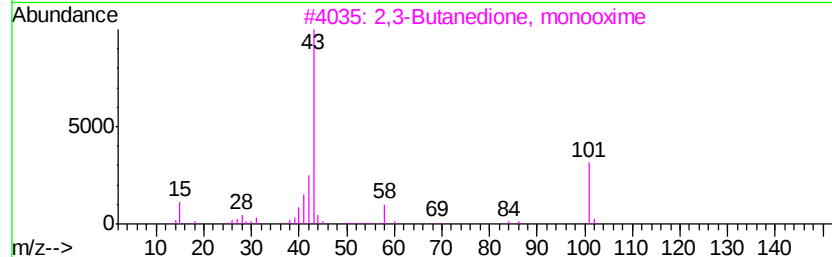
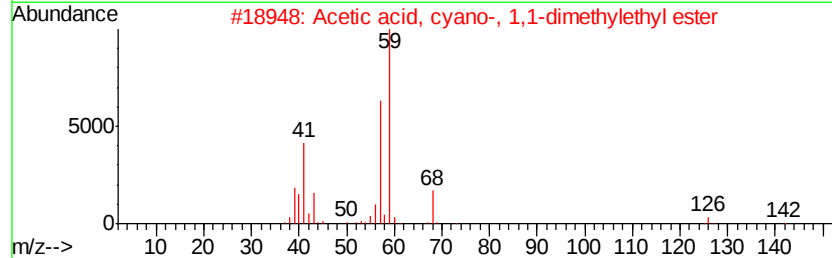
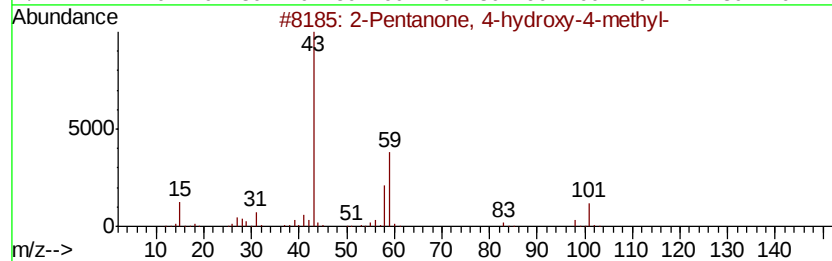
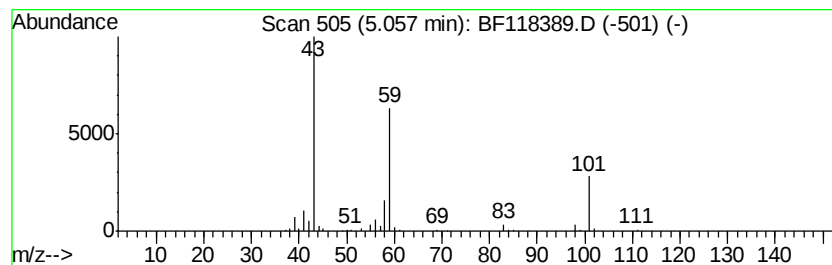
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	11.75 ng	416412	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5		Acetone	58	C3H6O	000067-64-1	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118389.D
Acq On : 30 Dec 2019 19:05
Operator : JU
Sample : K6442-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K615-WC-1

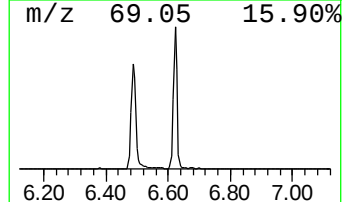
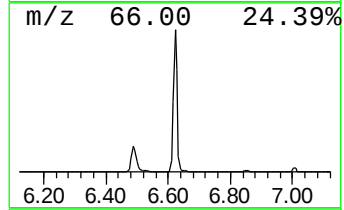
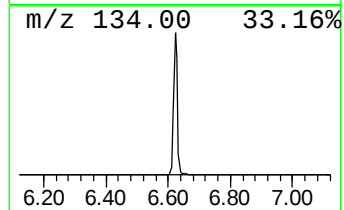
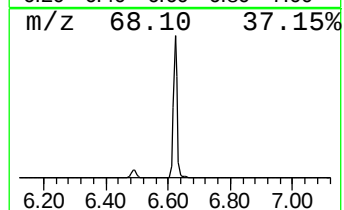
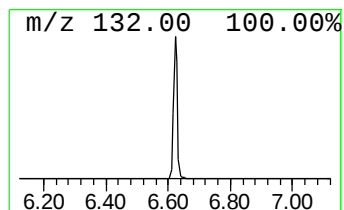
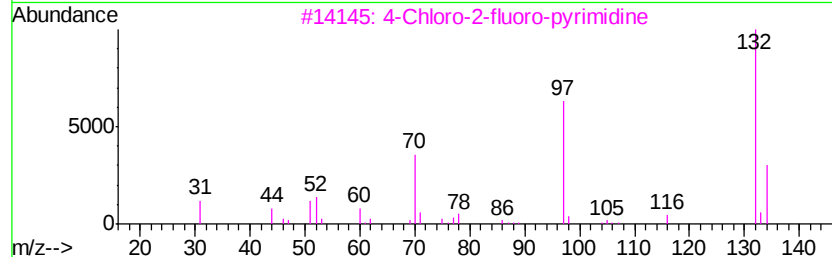
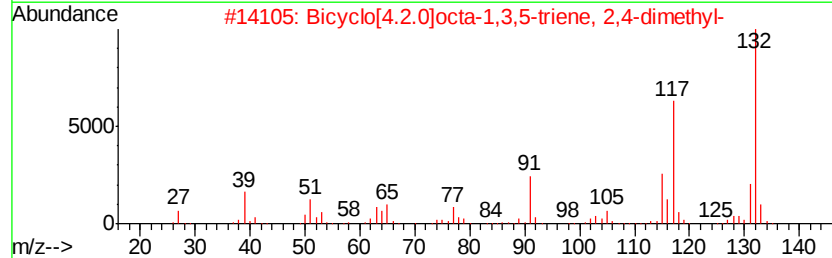
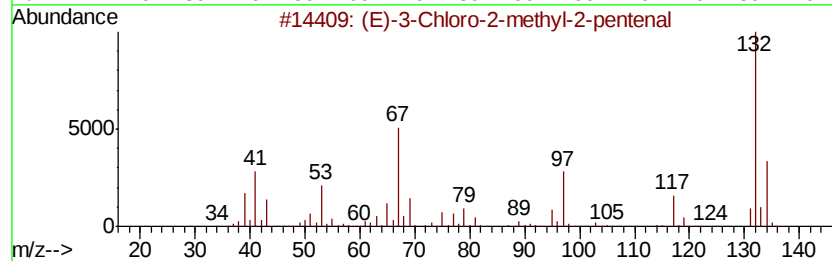
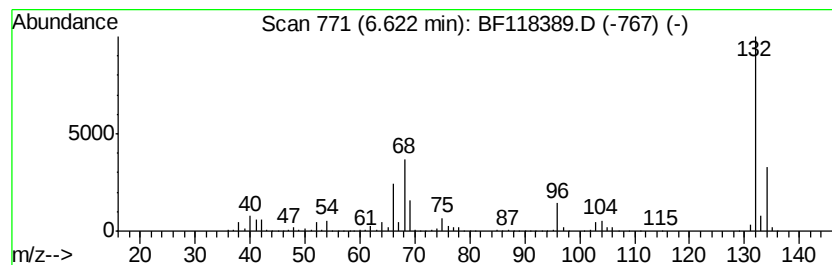
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown72.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	72.46 ng	2567640	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118389.D
Acq On : 30 Dec 2019 19:05
Operator : JU
Sample : K6442-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K615-WC-1

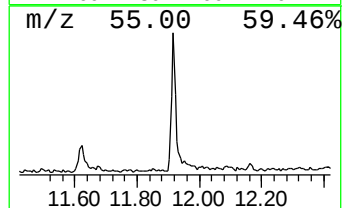
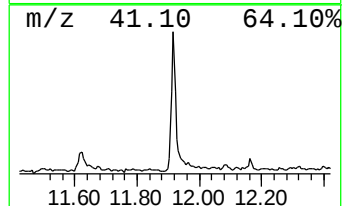
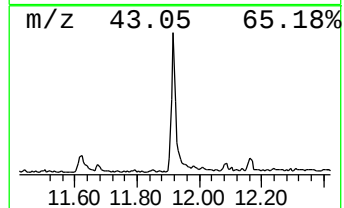
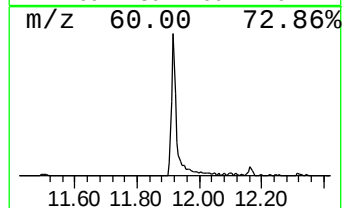
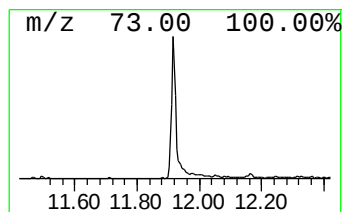
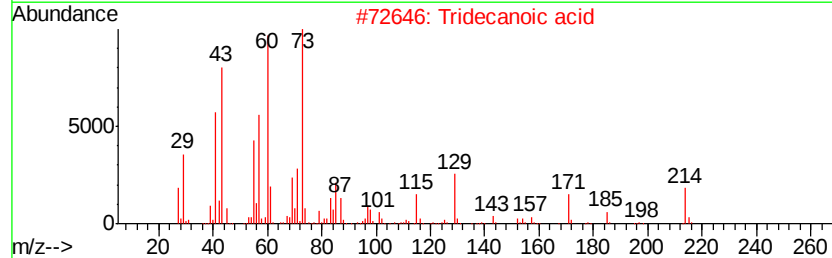
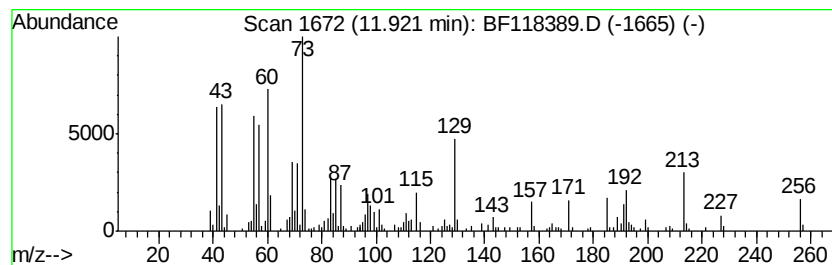
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	8.35 ng	492248	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Undecanoic acid	186	C11H22O2	000112-37-8	74
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118389.D
Acq On : 30 Dec 2019 19:05
Operator : JU
Sample : K6442-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K615-WC-1

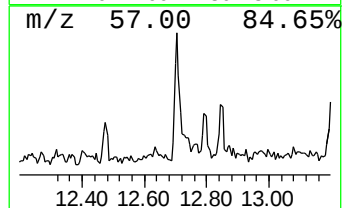
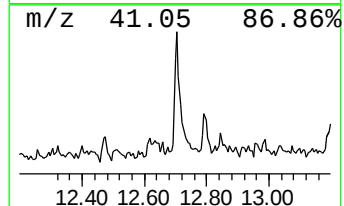
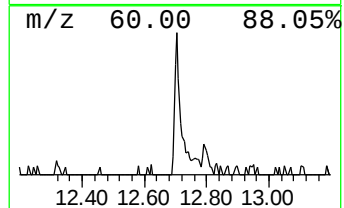
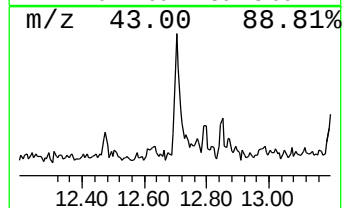
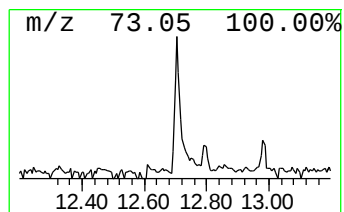
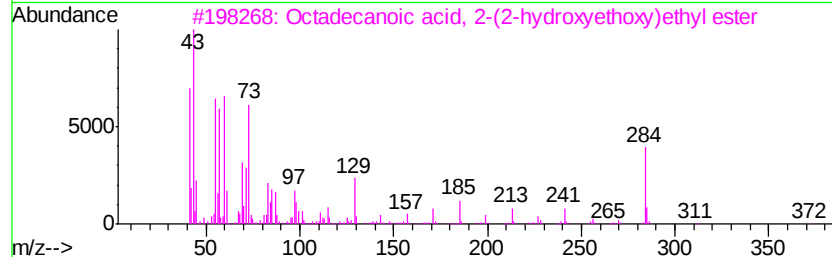
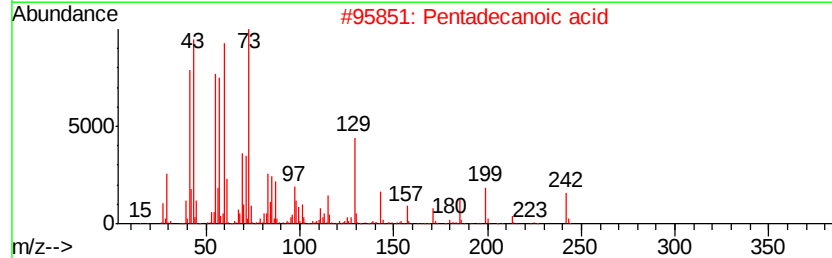
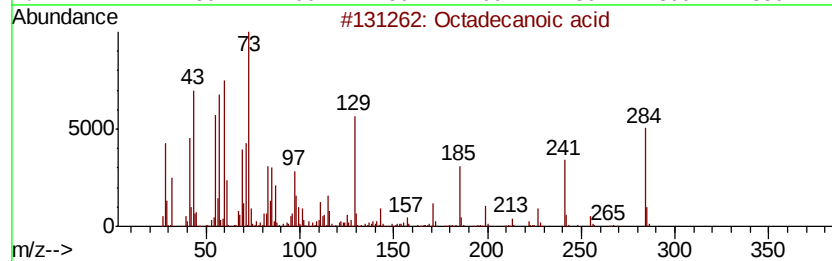
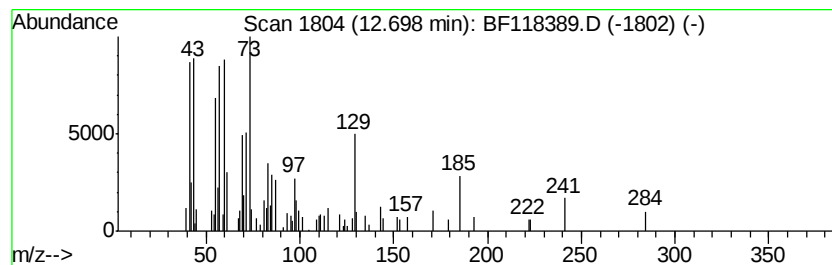
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.06 ng	121151	Phenanthrene-d10	11.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118389.D
Acq On : 30 Dec 2019 19:05
Operator : JU
Sample : K6442-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K615-WC-1

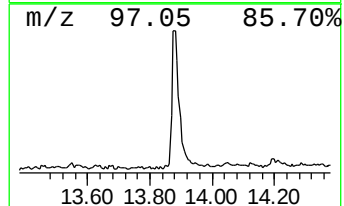
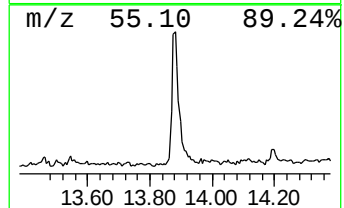
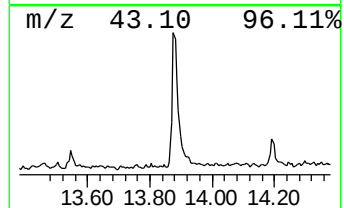
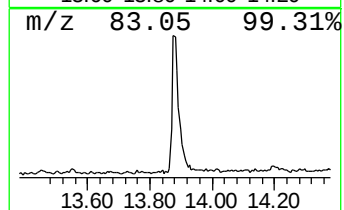
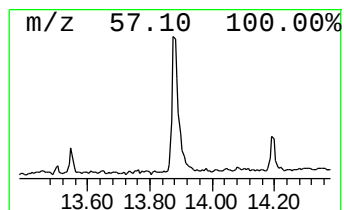
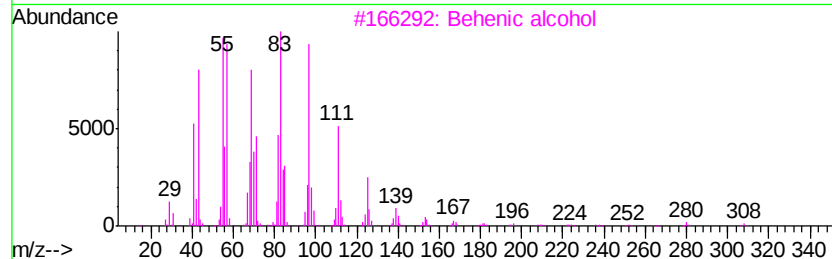
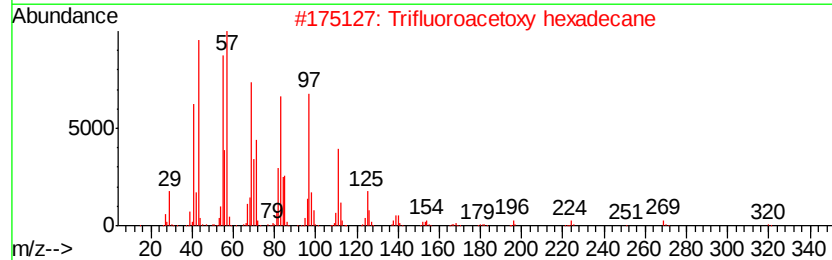
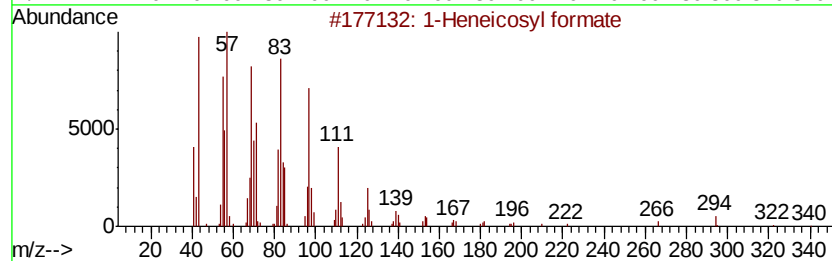
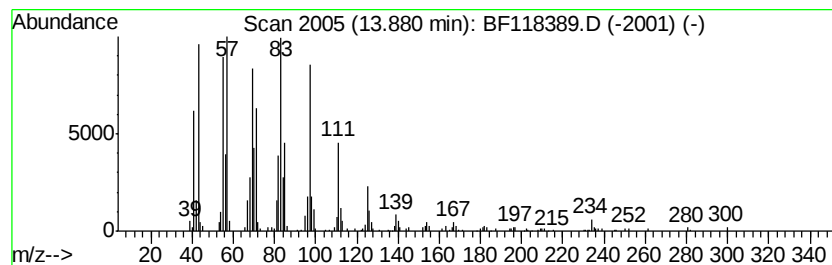
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	10.89 ng	549291	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		Behenic alcohol	326	C22H46O	000661-19-8	93
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5		5-Octadecene, (E)-	252	C18H36	007206-21-5	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118389.D
Acq On : 30 Dec 2019 19:05
Operator : JU
Sample : K6442-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

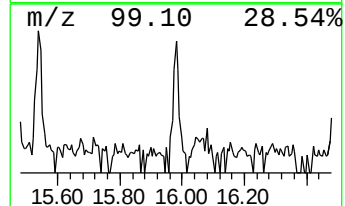
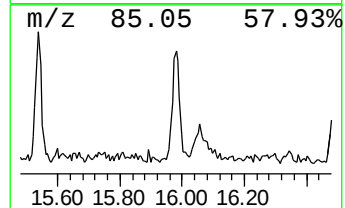
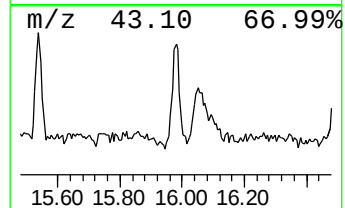
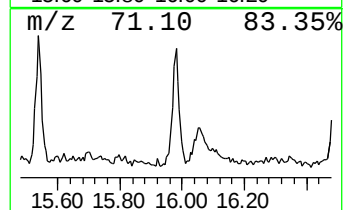
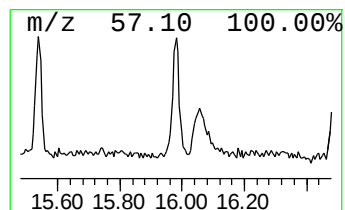
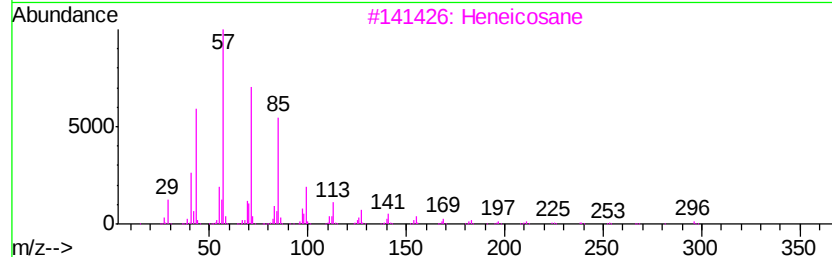
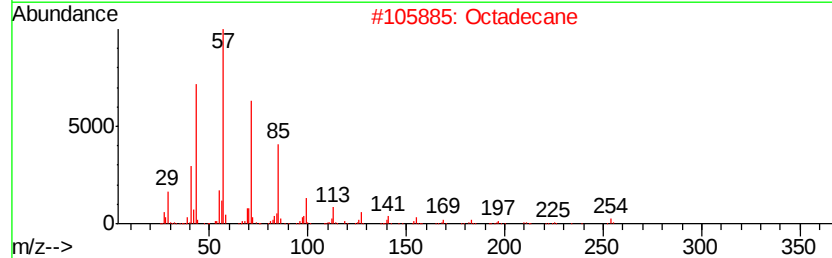
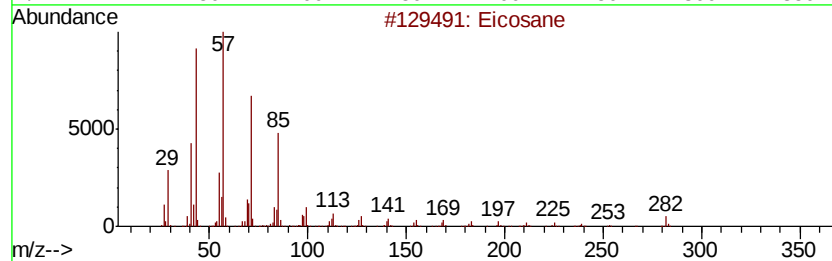
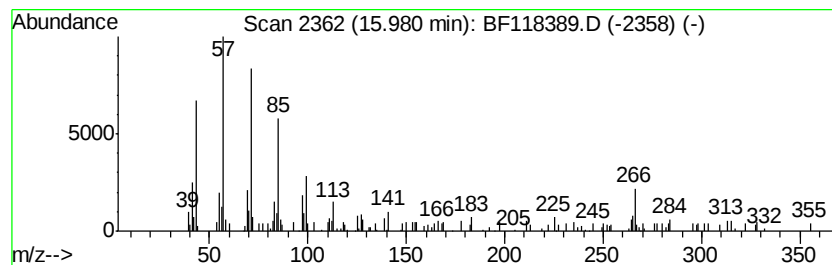
Instrument :
BNA_F
ClientSampleId :
K615-WC-1

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 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	2.03 ng	100219	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	92
2	Octadecane	254 C18H38	000593-45-3	86
3	Heneicosane	296 C21H44	000629-94-7	70
4	Hexacosane	366 C26H54	000630-01-3	62
5	Nonadecane	268 C19H40	000629-92-5	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118389.D
Acq On : 30 Dec 2019 19:05
Operator : JU
Sample : K6442-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K615-WC-1

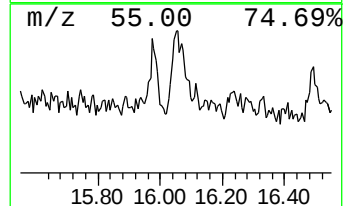
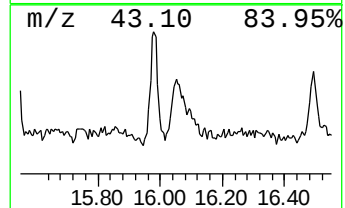
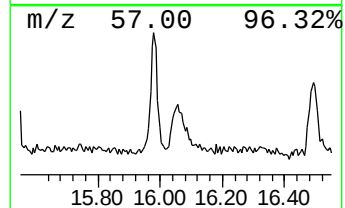
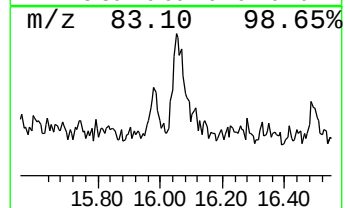
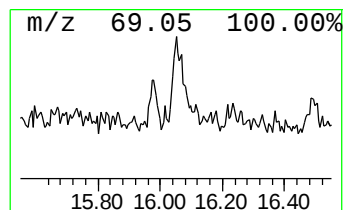
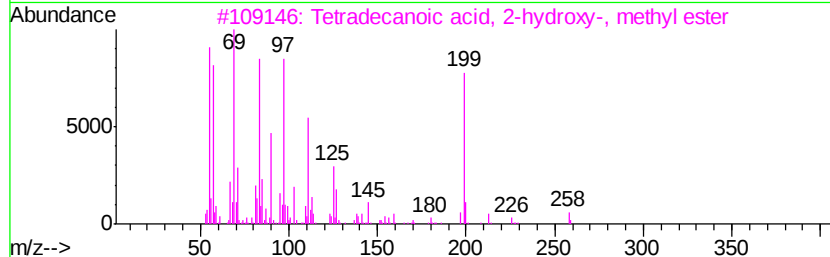
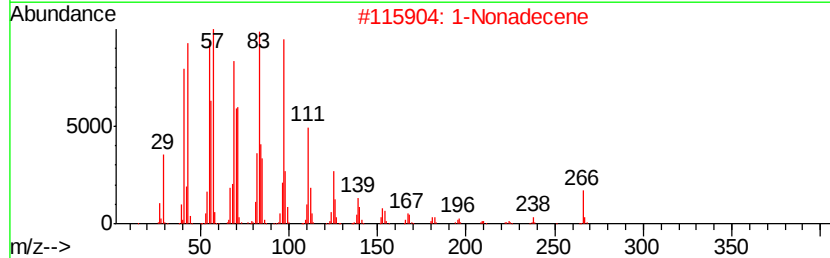
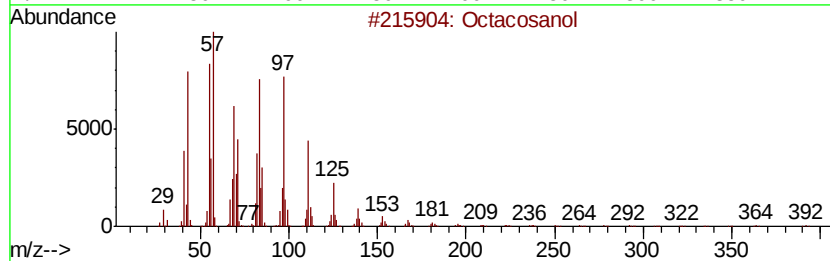
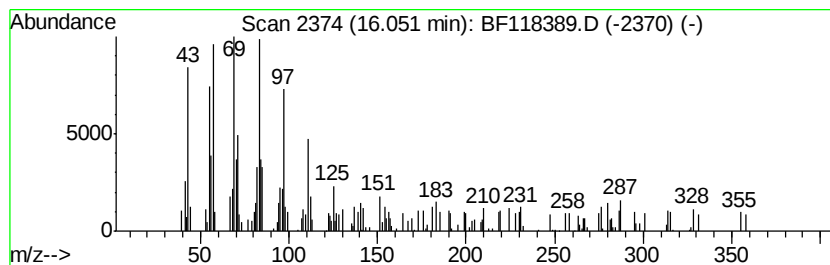
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	3.00 ng	148446	Perylene-d12	15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol		410	C28H58O	000557-61-9	86
2	1-Nonadecene		266	C19H38	018435-45-5	81
3	Tetradecanoic acid, 2-hydroxy-, ...		258	C15H30O3	056009-40-6	81
4	Cyclopentadecane		210	C15H30	000295-48-7	81
5	Z-5-Nonadecene		266	C19H38	1000131-11-8	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF123019\
Data File : BF118389.D
Acq On : 30 Dec 2019 19:05
Operator : JU
Sample : K6442-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K615-WC-1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.06	11.8	ng	416412	1	6.85	708685	20.0
unknown72.46	6.62	72.5	ng	2567640	1	6.85	708685	20.0
n-Hexadecanoic acid	11.92	8.3	ng	492248	4	11.39	1178930	20.0
Octadecanoic acid	12.70	2.1	ng	121151	4	11.39	1178930	20.0
1-Heneicosyl formate	13.88	10.9	ng	549291	5	14.05	1008970	20.0
Eicosane	15.98	2.0	ng	100219	6	15.54	989150	20.0
Octacosanol	16.05	3.0	ng	148446	6	15.54	989150	20.0