LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118313.D
Acq On : 26 Dec 2019 13:40
Operator : JU
Sample : K6417-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.875	299	304	312	rBV	116608	161279	4.90%	0.531%
2	4.551	414	419	425	rBB	85415	103109	3.13%	0.339%
3	5.045	499	503	515	rVB	358257	417388	12.69%	1.373%
4	5.428	564	568	570	rBV	144975	156217	4.75%	0.514%
5	5.457	570	573	589	rVB	2169319	2174857	66.10%	7.156%
6	5.687	609	612	616	rBV	99491	89816	2.73%	0.296%
7	6.481	743	747	760	rBV	2598448	2367713	71.97%	7.791%
8	6.616	766	770	774	rBV	2919446	2497564	75.91%	8.218%
9	6.675	777	780	784	rVB	60507	60262	1.83%	0.198%
10	6.845	806	809	816	rVB	699598	637233	19.37%	2.097%
11	7.004	832	836	846	rBV	2413292	1945339	59.13%	6.401%
12	7.416	901	906	915	rBV	1455053	1445741	43.94%	4.757%
13	8.133	1025	1028	1035	rBV	963502	822257	24.99%	2.706%
14	9.216	1208	1212	1215	rBV	3396590	3004694	91.33%	9.887%
15	9.610	1275	1279	1283	rBV	166225	162556	4.94%	0.535%
16	9.898	1324	1328	1331	rBV	1148994	1011698	30.75%	3.329%
17	10.545	1433	1438	1444	rBV2	24479	41723	1.27%	0.137%
18	10.686	1459	1462	1474	rVB	2230416	2147906	65.29%	7.068%
19	10.810	1478	1483	1487	rBV2	72643	96796	2.94%	0.319%
20	11.245	1554	1557	1560	rBV2	52135	47598	1.45%	0.157%
21	11.280	1560	1563	1570	rVB4	29188	44323	1.35%	0.146%
22	11.386	1578	1581	1584	rBV	1238158	1126709	34.25%	3.707%
23	11.410	1584	1585	1589	rVB	208667	147586	4.49%	0.486%
24	11.627	1618	1622	1625	rBV5	34247	59751	1.82%	0.197%
25	11.674	1627	1630	1633	rVV3	54861	57979	1.76%	0.191%
26	11.721	1636	1638	1644	rVB5	26437	43430	1.32%	0.143%
27	11.892	1664	1667	1668	rBV	44514	39117	1.19%	0.129%
28	11.916	1668	1671	1677	rVB2	382339	422318	12.84%	1.390%
29	12.004	1683	1686	1688	rBV2	69154	62964	1.91%	0.207%
30	12.186	1715	1717	1720	rBV2	59658	50485	1.53%	0.166%
31	12.221	1720	1723	1727	rVB4	42484	50103	1.52%	0.165%
32	12.445	1758	1761	1763	rBV	77277	72706	2.21%	0.239%
33	12.474	1763	1766	1769	rVV3	69705	81840	2.49%	0.269%
34	12.533	1773	1776	1780	rVB4	41638	54407	1.65%	0.179%

LSC Area Percent Report

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Acq On : 26 Dec 2019 13:40
Operator : JU
Sample : K6417-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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	12.610	1785	1789	1793	rBV	343821	341914	10.39%	1.125%
36	12.704	1802	1805	1813	rBV6	121539	181715	5.52%	0.598%
37	12.839	1822	1828	1834	rBV	321523	341645	10.38%	1.124%
38	12.980	1848	1852	1855	rBV	3947793	3290026	100.00%	10.826%
39	13.057	1862	1865	1872	rVB5	35582	60295	1.83%	0.198%
40	13.268	1899	1901	1904	rVB2	47278	43042	1.31%	0.142%
41	13.545	1946	1948	1951	rVB2	51017	41751	1.27%	0.137%
42	13.680	1969	1971	1976	rVB	58262	49057	1.49%	0.161%
43	13.874	2001	2004	2014	rVB2	436179	592070	18.00%	1.948%
44	14.039	2025	2032	2035	rBV2	1012003	1138158	34.59%	3.745%
45	14.068	2035	2037	2045	rVB	167883	179790	5.46%	0.592%
46	14.192	2056	2058	2068	rVB3	114484	149118	4.53%	0.491%
47	14.504	2107	2111	2117	rBV3	142615	206905	6.29%	0.681%
48	14.809	2160	2163	2167	rVB	133810	131033	3.98%	0.431%
49	15.092	2208	2211	2214	rBV	117125	158734	4.82%	0.522%
50	15.151	2218	2221	2227	rVB	129579	151914	4.62%	0.500%
51	15.398	2260	2263	2267	rVB	71740	90608	2.75%	0.298%
52	15.462	2271	2274	2280	rVV	123624	164985	5.01%	0.543%
53	15.527	2280	2285	2297	rVB	725881	1044770	31.76%	3.438%
54	15.974	2358	2361	2367	rVB	87830	131718	4.00%	0.433%
55	17.027	2536	2540	2547	rVB2	49913	97255	2.96%	0.320%
56	17.480	2612	2617	2624	rVB	45873	98648	3.00%	0.325%

Sum of corrected areas: 30390615

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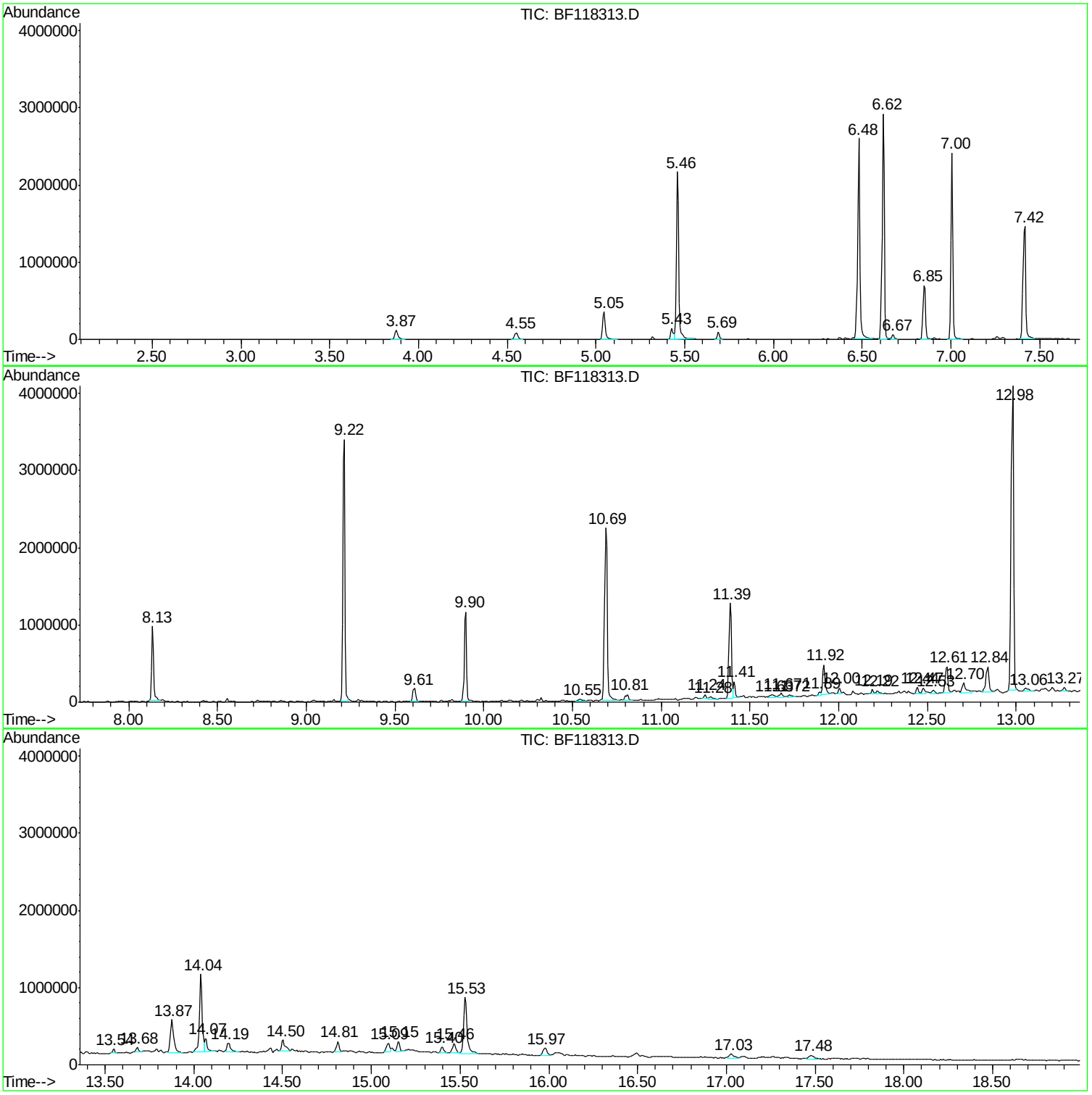
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118313.D
Acq On : 26 Dec 2019 13:40
Operator : JU
Sample : K6417-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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

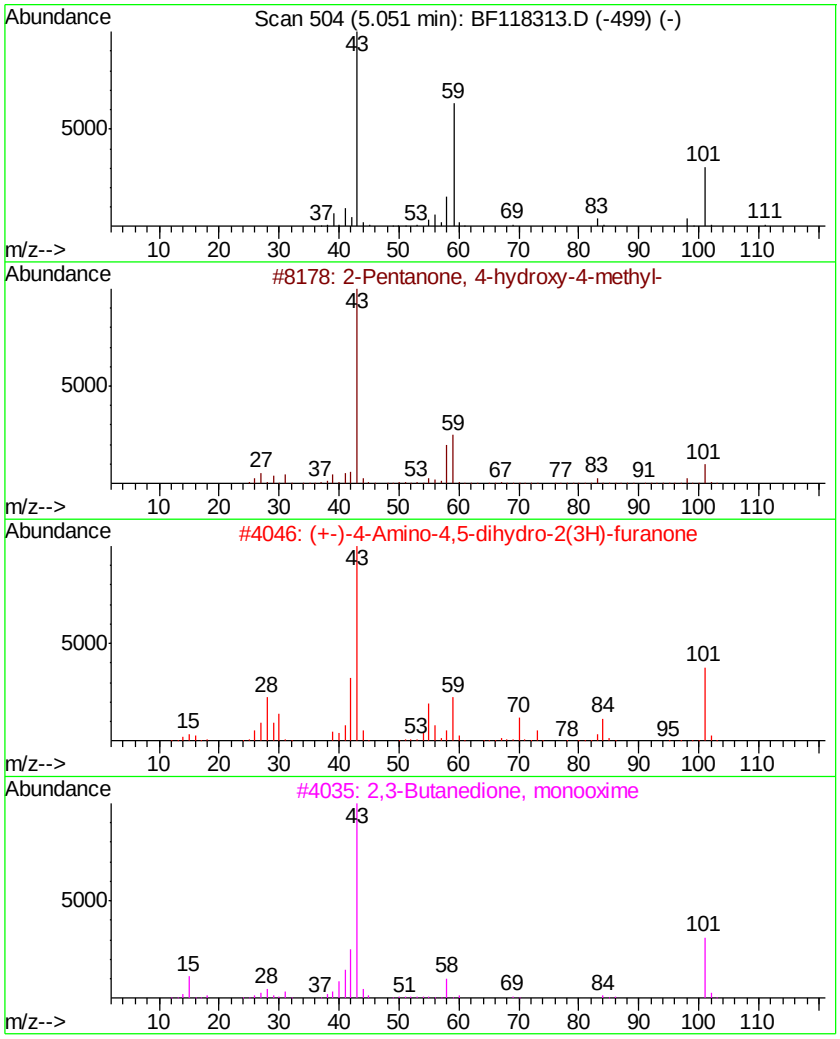
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

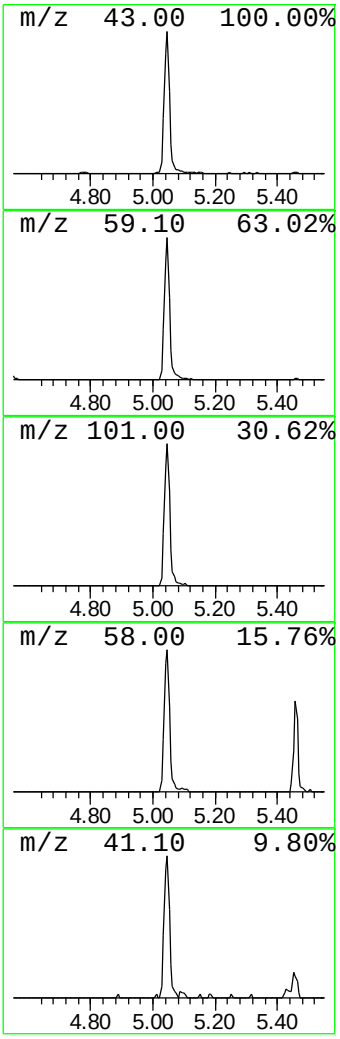
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	13.10 ng	417388	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	64
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118313.D
Acq On : 26 Dec 2019 13:40
Operator : JU
Sample : K6417-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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

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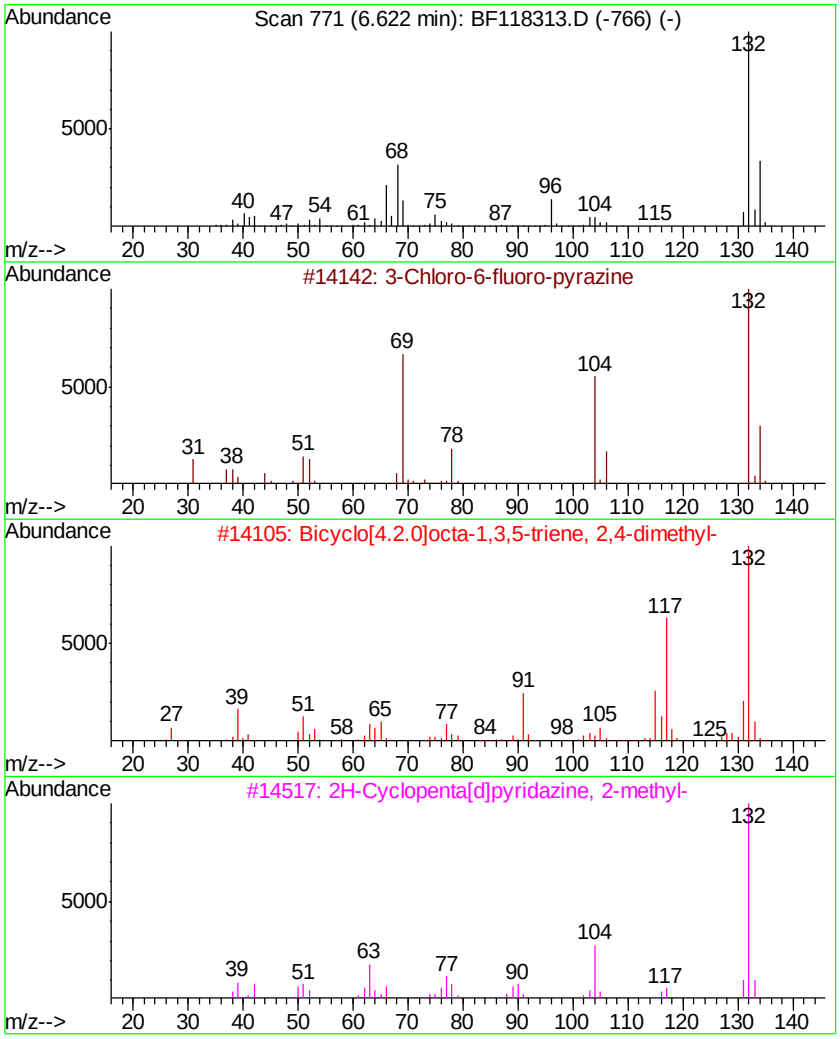
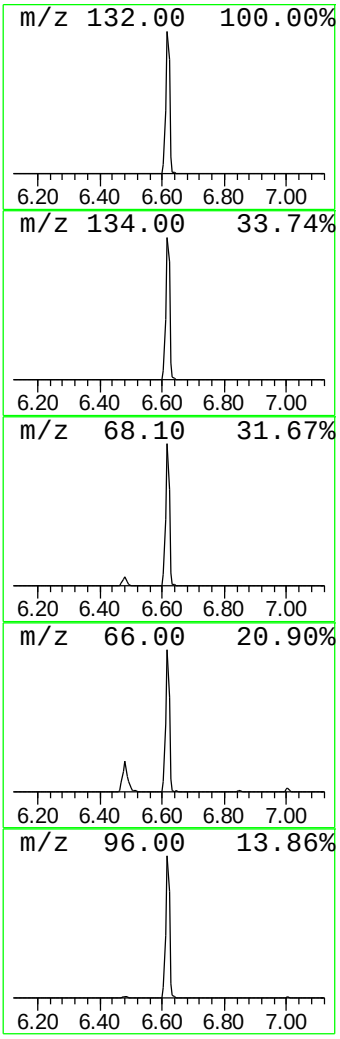
Peak Number 5 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	78.39 ng	2497560	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	35
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	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\BF122619\
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Acq On : 26 Dec 2019 13:40
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Sample : K6417-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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

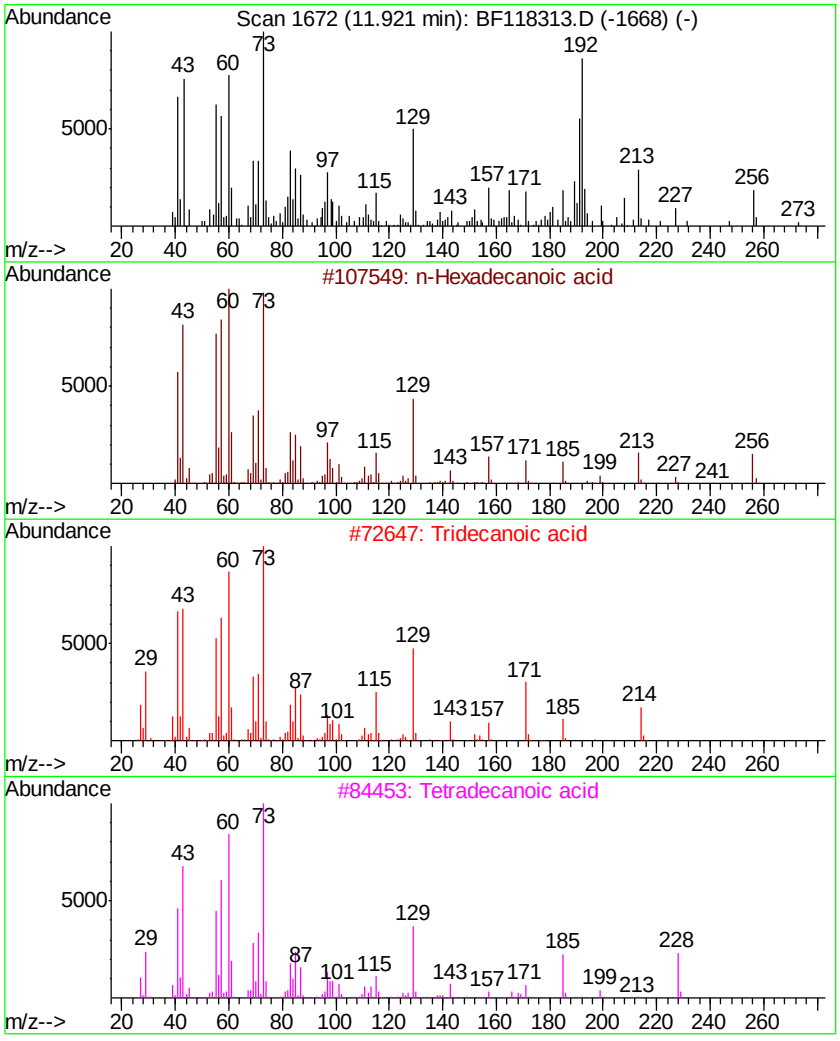
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

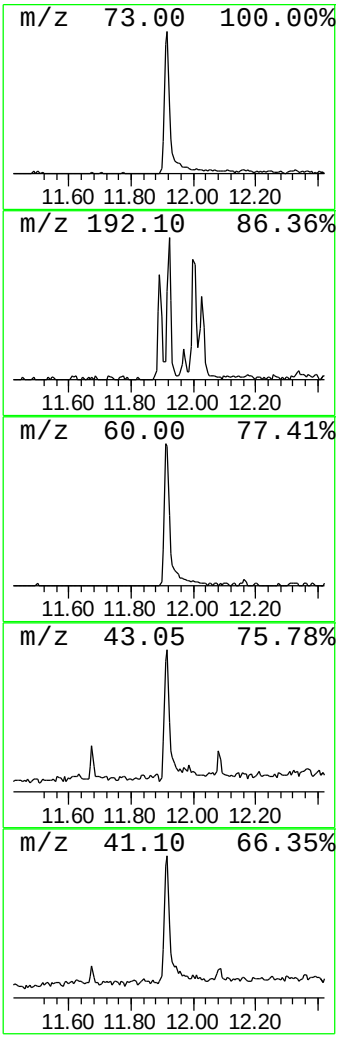
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	7.50 ng	422318	Phenanthrene-d10	11.39

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	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Ether, dodecyl isopropyl	228	C15H32O	029379-42-8	25





Library Search Compound Report

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Sample : K6417-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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

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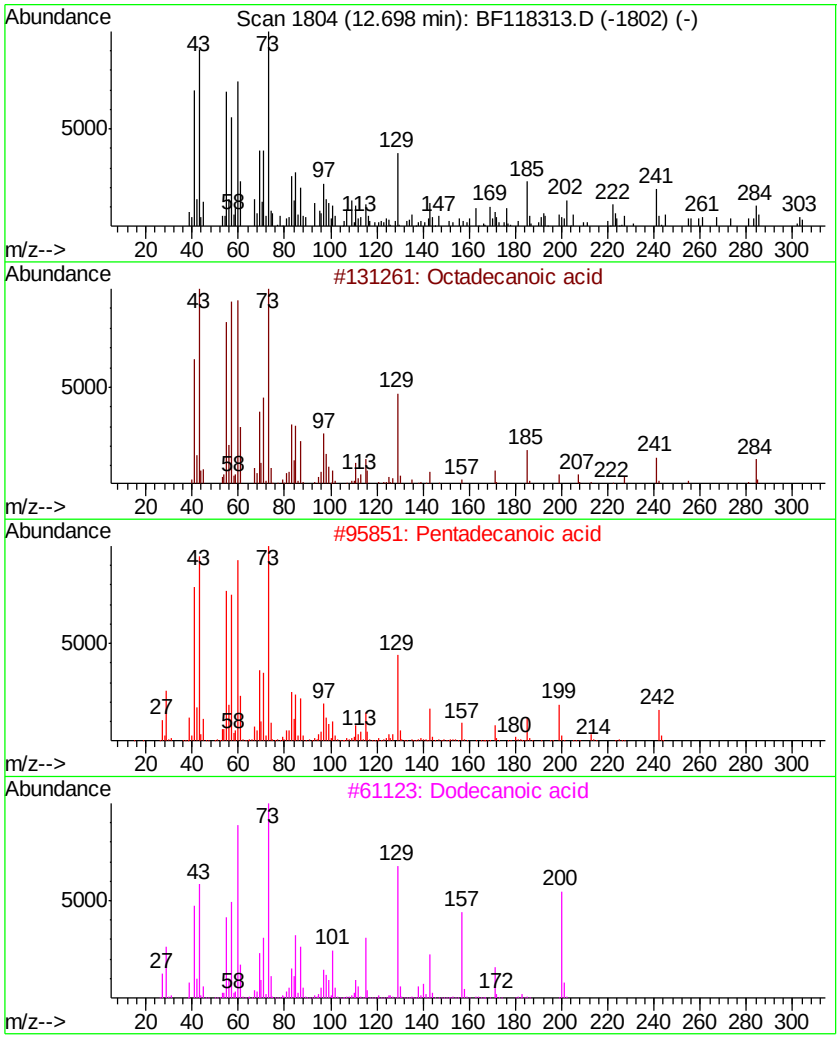
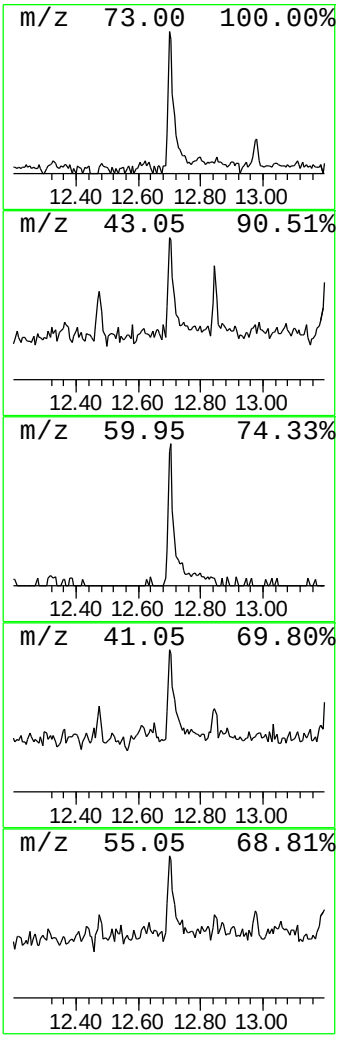
Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	3.23 ng	181715	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Dodecanoic acid	200	C12H24O2	000143-07-7	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Sample : K6417-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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

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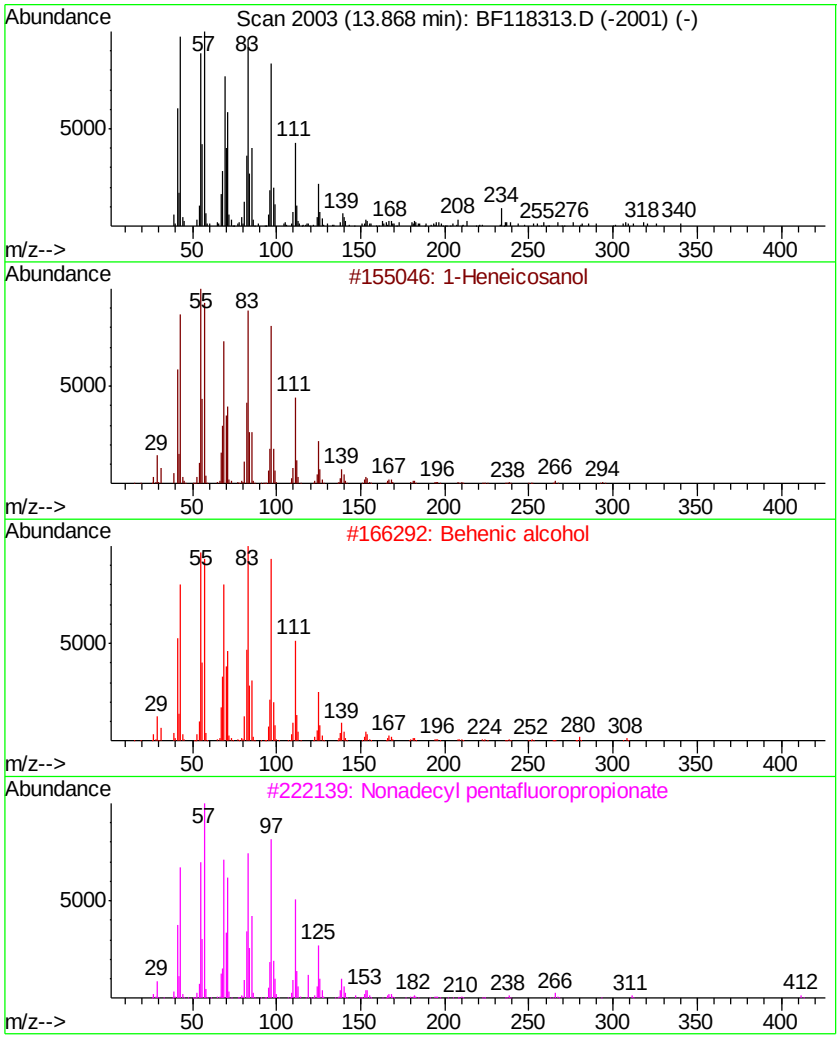
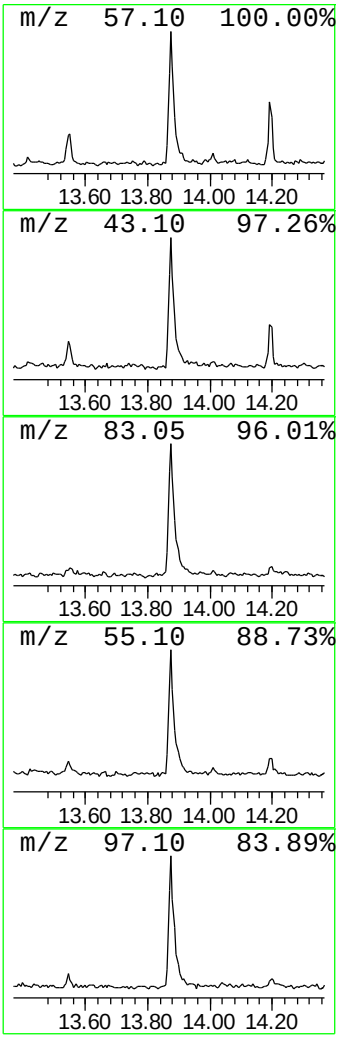
Peak Number 9 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	10.40 ng	592070	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
4	1-Heptacosanol	396	C27H56O	002004-39-9	90
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90





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Instrument : BNA_F
ClientSampleId : TP-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

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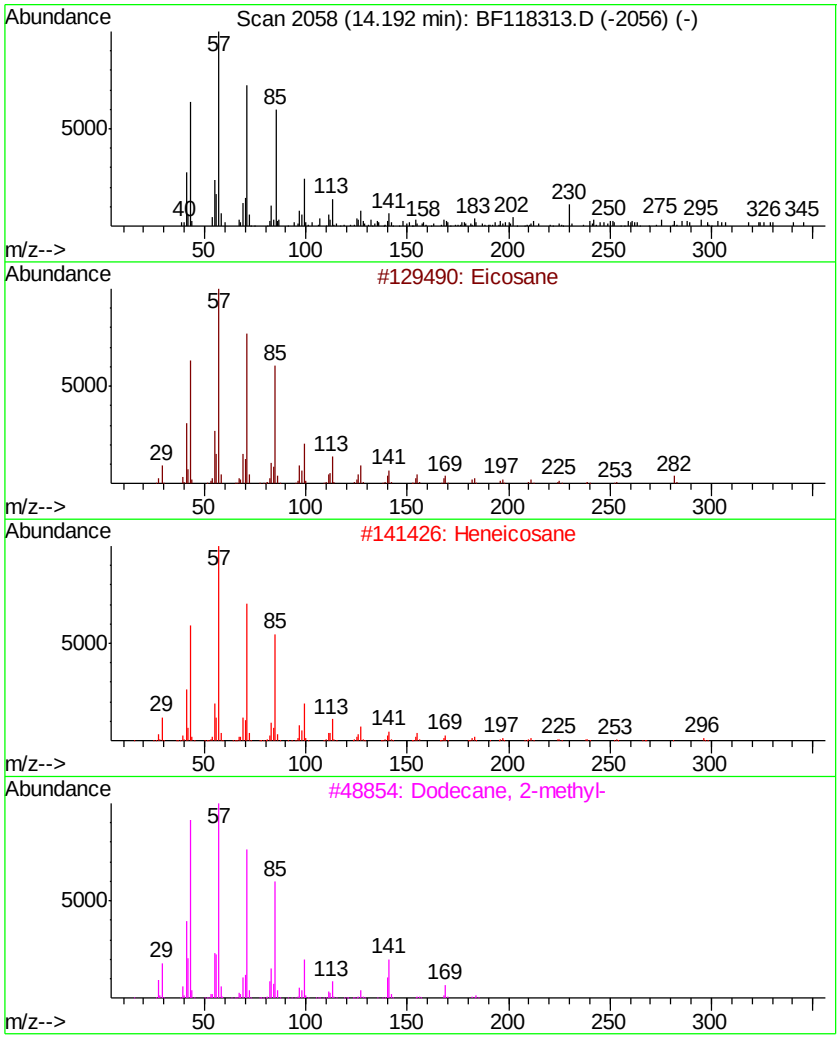
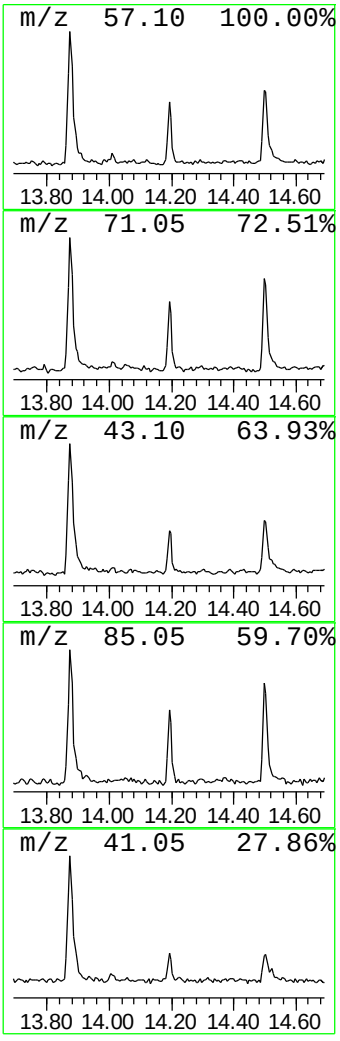
Peak Number 10 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.62 ng	149118	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	87
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	83
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	80
5	Heptadecane	240	C17H36	000629-78-7	76





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Misc :
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Instrument : BNA_F
ClientSampleId : TP-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

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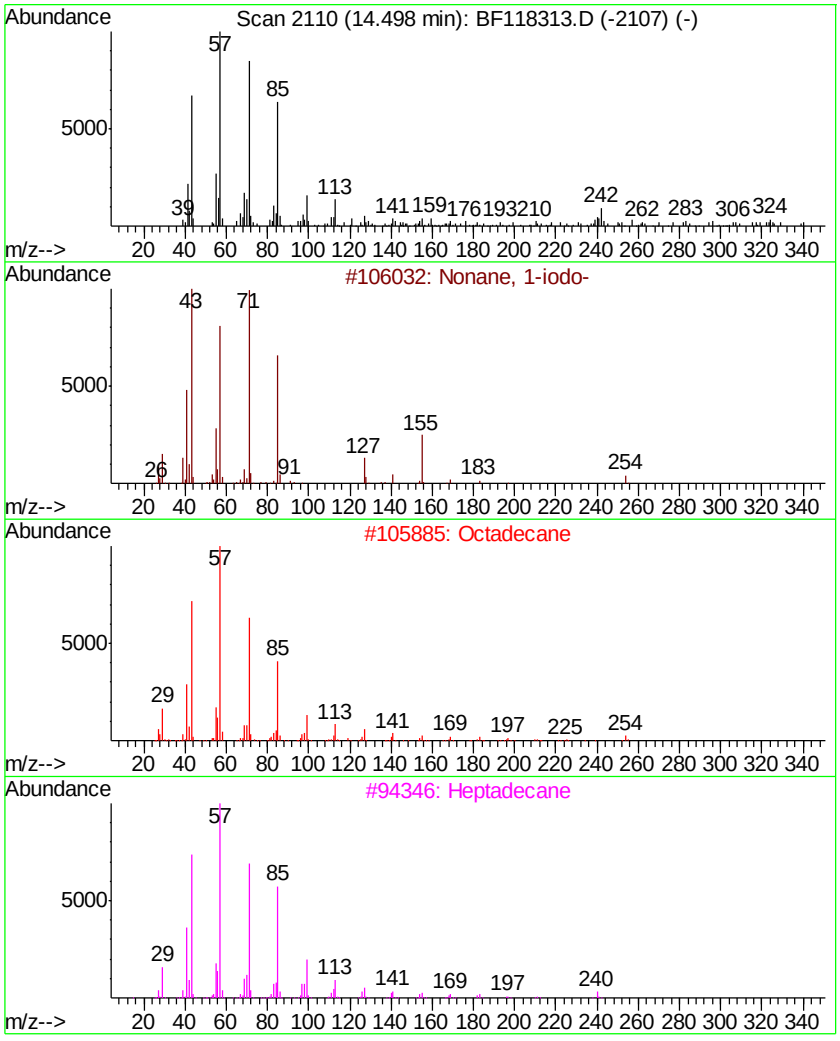
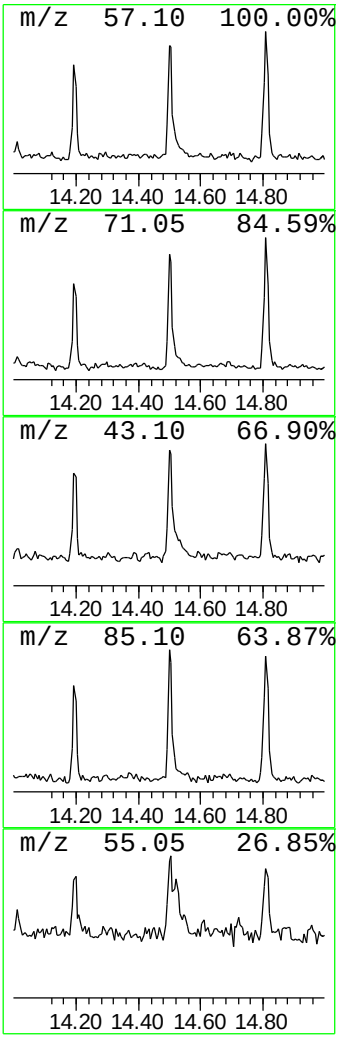
Peak Number 11 Nonane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	3.64 ng	206905	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 1-iodo-	254	C9H19I	004282-42-2	92
2	Octadecane	254	C18H38	000593-45-3	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Hexacosane	366	C26H54	000630-01-3	87
5	Eicosane	282	C20H42	000112-95-8	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118313.D
Acq On : 26 Dec 2019 13:40
Operator : JU
Sample : K6417-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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

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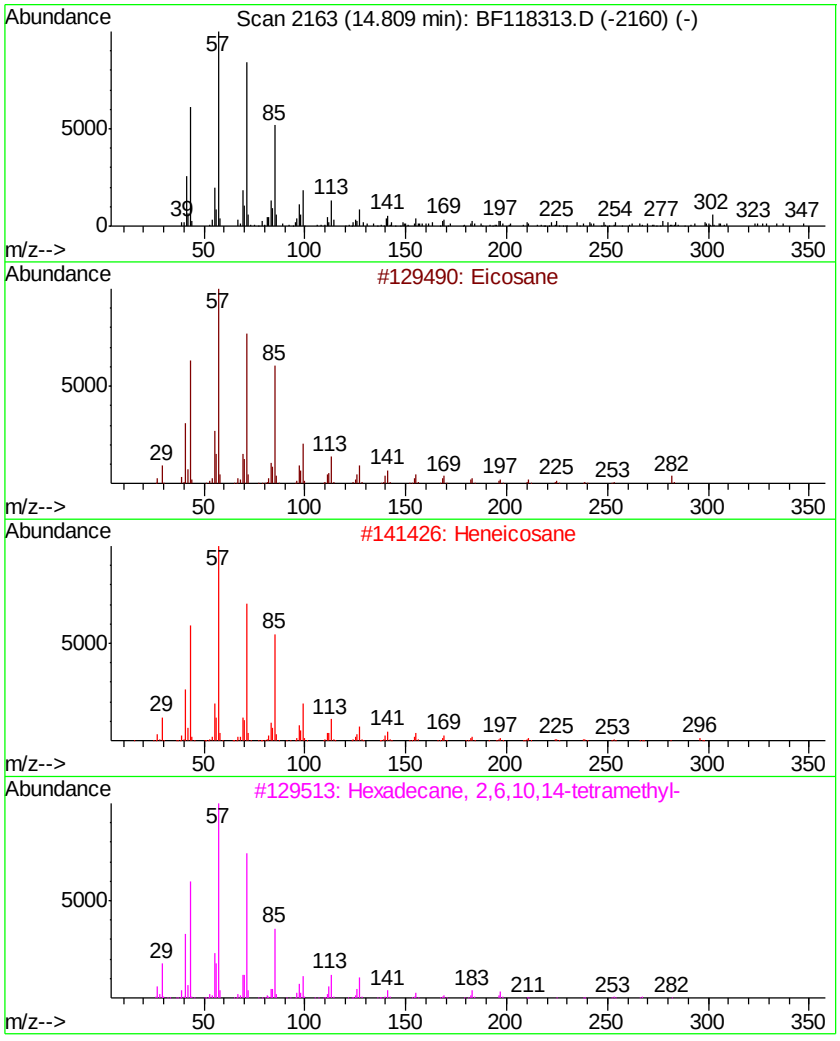
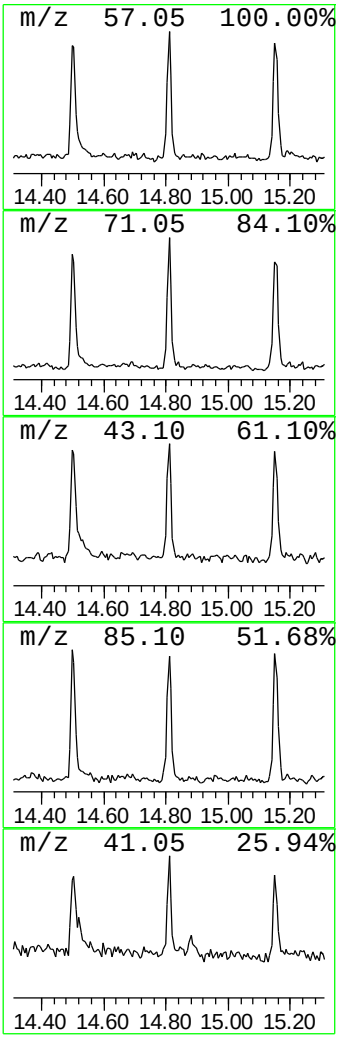
Peak Number 12 Heneicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.51 ng	131033	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118313.D
Acq On : 26 Dec 2019 13:40
Operator : JU
Sample : K6417-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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

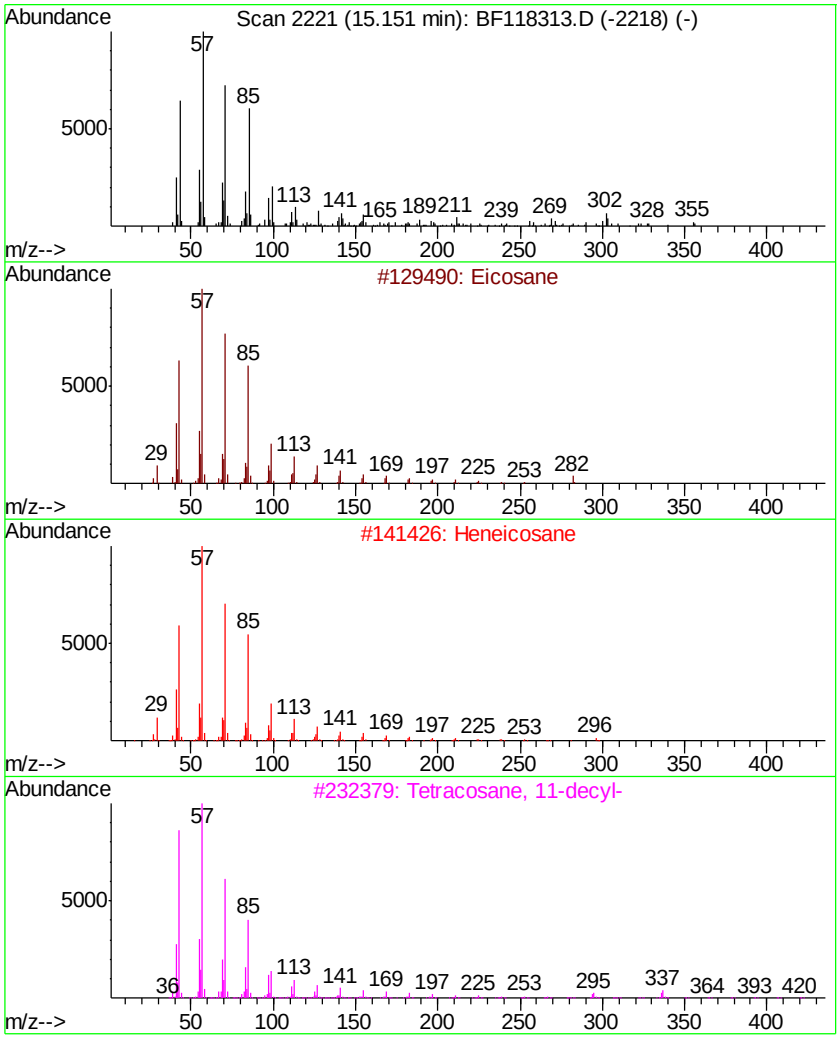
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

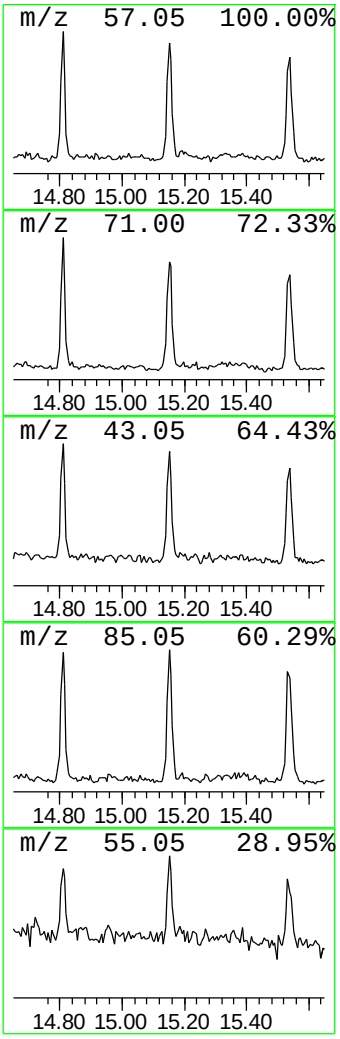
****

Peak Number 13 Tetracosane, 11-decyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	2.91 ng	151914	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118313.D
Acq On : 26 Dec 2019 13:40
Operator : JU
Sample : K6417-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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

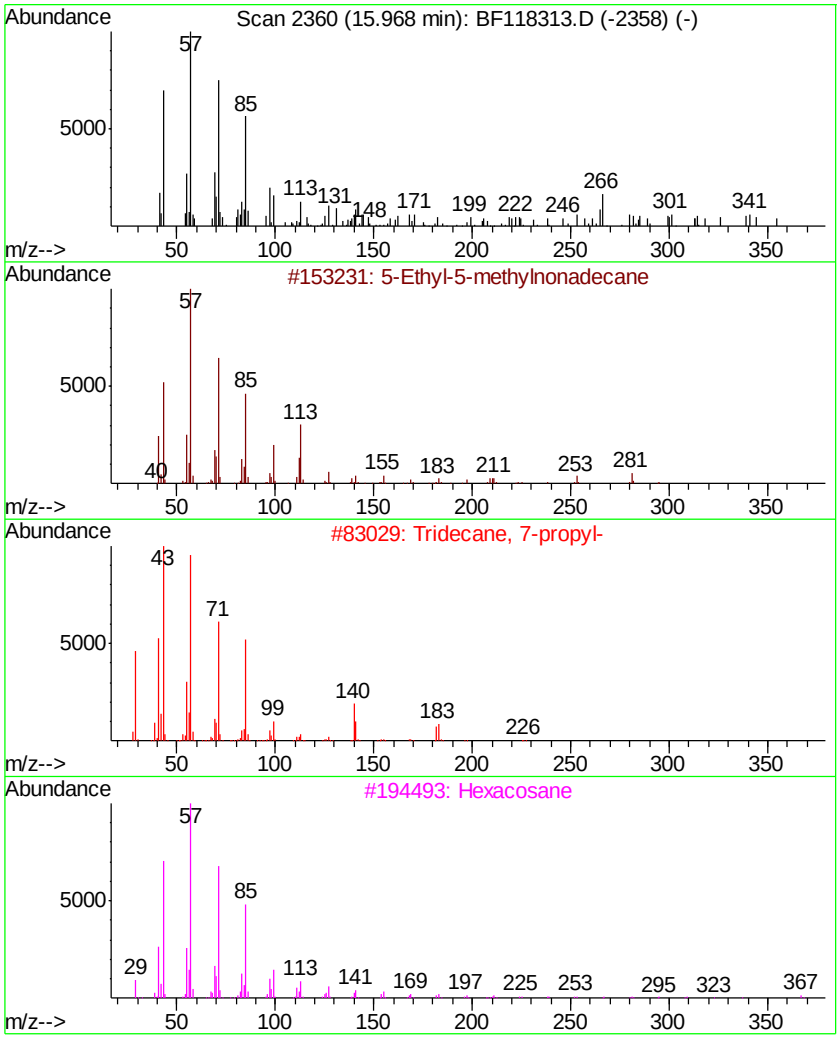
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

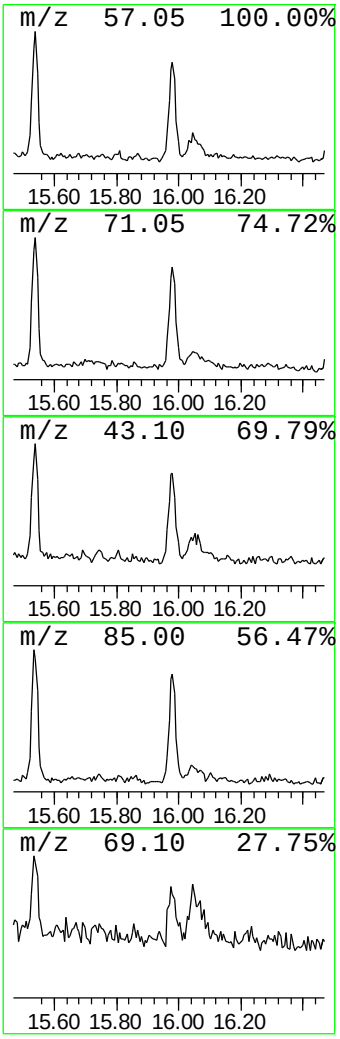
****

Peak Number 14 5-Ethyl-5-methylnonadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.52 ng	131718	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	72
2	Tridecane, 7-propyl-	226	C16H34	055045-09-5	62
3	Hexacosane	366	C26H54	000630-01-3	62
4	2-methyloctacosane	408	C29H60	1000376-72-8	62
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122619\
Data File : BF118313.D
Acq On : 26 Dec 2019 13:40
Operator : JU
Sample : K6417-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	13.1	ng	417388	1	6.85	637233	20.0
unknown6.62	6.62	78.4	ng	2497560	1	6.85	637233	20.0
n-Hexadecanoic acid	11.92	7.5	ng	422318	4	11.39	1126710	20.0
Octadecanoic acid	12.70	3.2	ng	181715	4	11.39	1126710	20.0
1-Heneicosanol	13.87	10.4	ng	592070	5	14.04	1138160	20.0
Eicosane	14.19	2.6	ng	149118	5	14.04	1138160	20.0
Nonane, 1-iodo-	14.50	3.6	ng	206905	5	14.04	1138160	20.0
Heneicosane	14.81	2.5	ng	131033	6	15.53	1044770	20.0
Tetracosane, 11-d...	15.15	2.9	ng	151914	6	15.53	1044770	20.0
5-Ethyl-5-methyln...	15.97	2.5	ng	131718	6	15.53	1044770	20.0