LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118332.D
Acq On : 26 Dec 2019 22:36
Operator : JU
Sample : K6436-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K009-WC-2

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	5.040	499	502	511	rBV	165600	180465	12.24%	1.238%
2	5.463	570	574	593	rVB	936884	940148	63.79%	6.448%
3	6.481	744	747	762	rBV	1095742	1105555	75.01%	7.583%
4	6.622	767	771	778	rVV	1384510	1151777	78.15%	7.900%
5	6.851	807	810	817	rBV	525724	421165	28.58%	2.889%
6	7.004	833	836	845	rBV	997538	944175	64.06%	6.476%
7	7.416	902	906	916	rBV	675843	617414	41.89%	4.235%
8	7.657	944	947	953	rVB3	14916	18998	1.29%	0.130%
9	8.139	1023	1029	1036	rBV	628770	584519	39.66%	4.009%
10	9.216	1208	1212	1221	rBV	1859414	1473822	100.00%	10.109%
11	9.292	1222	1225	1228	rVB3	29122	28110	1.91%	0.193%
12	9.369	1235	1238	1240	rVB	21331	19503	1.32%	0.134%
13	9.486	1253	1258	1263	rBV7	23284	30124	2.04%	0.207%
14	9.557	1268	1270	1272	rVV	25297	24743	1.68%	0.170%
15	9.610	1276	1279	1282	rVB	90082	84470	5.73%	0.579%
16	9.763	1302	1305	1307	rBV3	23393	24879	1.69%	0.171%
17	9.898	1325	1328	1332	rVB	761342	627836	42.60%	4.306%
18	10.004	1343	1346	1350	rBV5	20800	24716	1.68%	0.170%
19	10.104	1360	1363	1367	rVB2	24095	24528	1.66%	0.168%
20	10.145	1367	1370	1374	rVB3	29544	29723	2.02%	0.204%
21	10.216	1379	1382	1385	rBV2	26473	33195	2.25%	0.228%
22	10.304	1394	1397	1399	rBV4	22196	26385	1.79%	0.181%
23	10.327	1399	1401	1403	rVB	36333	27752	1.88%	0.190%
24	10.545	1435	1438	1444	rVB5	28137	44538	3.02%	0.305%
25	10.598	1444	1447	1450	rBV5	14261	21738	1.47%	0.149%
26	10.692	1460	1463	1474	rBV	717050	657348	44.60%	4.509%
27	10.816	1479	1484	1489	rVB2	67832	106163	7.20%	0.728%
28	10.892	1494	1497	1499	rBV4	19856	20825	1.41%	0.143%
29	11.251	1555	1558	1560	rBV	44157	34896	2.37%	0.239%
30	11.280	1560	1563	1569	rVB4	51336	64213	4.36%	0.440%
31	11.392	1579	1582	1585	rBV	712793	611516	41.49%	4.194%
32	11.416	1585	1586	1589	rVB	78545	56509	3.83%	0.388%
33	11.680	1628	1631	1634	rVB2	43268	42111	2.86%	0.289%
34	11.733	1637	1640	1644	rVB4	32689	48501	3.29%	0.333%

LSC Area Percent Report

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Operator : JU
Sample : K6436-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K009-WC-2

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	11.916	1668	1671	1679	rVB5	153164	181606	12.32%	1.246%
36	12.010	1684	1687	1689	rVV2	29110	26703	1.81%	0.183%
37	12.033	1689	1691	1693	rVB2	41553	28199	1.91%	0.193%
38	12.086	1697	1700	1702	rBV	63941	57218	3.88%	0.392%
39	12.133	1705	1708	1710	rBV2	29097	34381	2.33%	0.236%
40	12.192	1716	1718	1720	rBV2	31838	32749	2.22%	0.225%
41	12.327	1738	1741	1745	rBV3	36293	50964	3.46%	0.350%
42	12.451	1759	1762	1764	rBV	56634	56117	3.81%	0.385%
43	12.474	1764	1766	1770	rVB2	86345	79002	5.36%	0.542%
44	12.615	1787	1790	1794	rBV	267894	332032	22.53%	2.277%
45	12.845	1826	1829	1835	rVB	294848	306214	20.78%	2.100%
46	12.980	1849	1852	1861	rVB	1600773	1397127	94.80%	9.583%
47	13.551	1947	1949	1952	rVB	106682	90339	6.13%	0.620%
48	13.880	2003	2005	2011	rVB2	246143	286518	19.44%	1.965%
49	14.051	2030	2034	2036	rBV2	576793	662184	44.93%	4.542%
50	14.198	2057	2059	2062	rBV	172397	176062	11.95%	1.208%
51	15.545	2285	2288	2292	rBV2	521622	630135	42.76%	4.322%

Sum of corrected areas: 14579910

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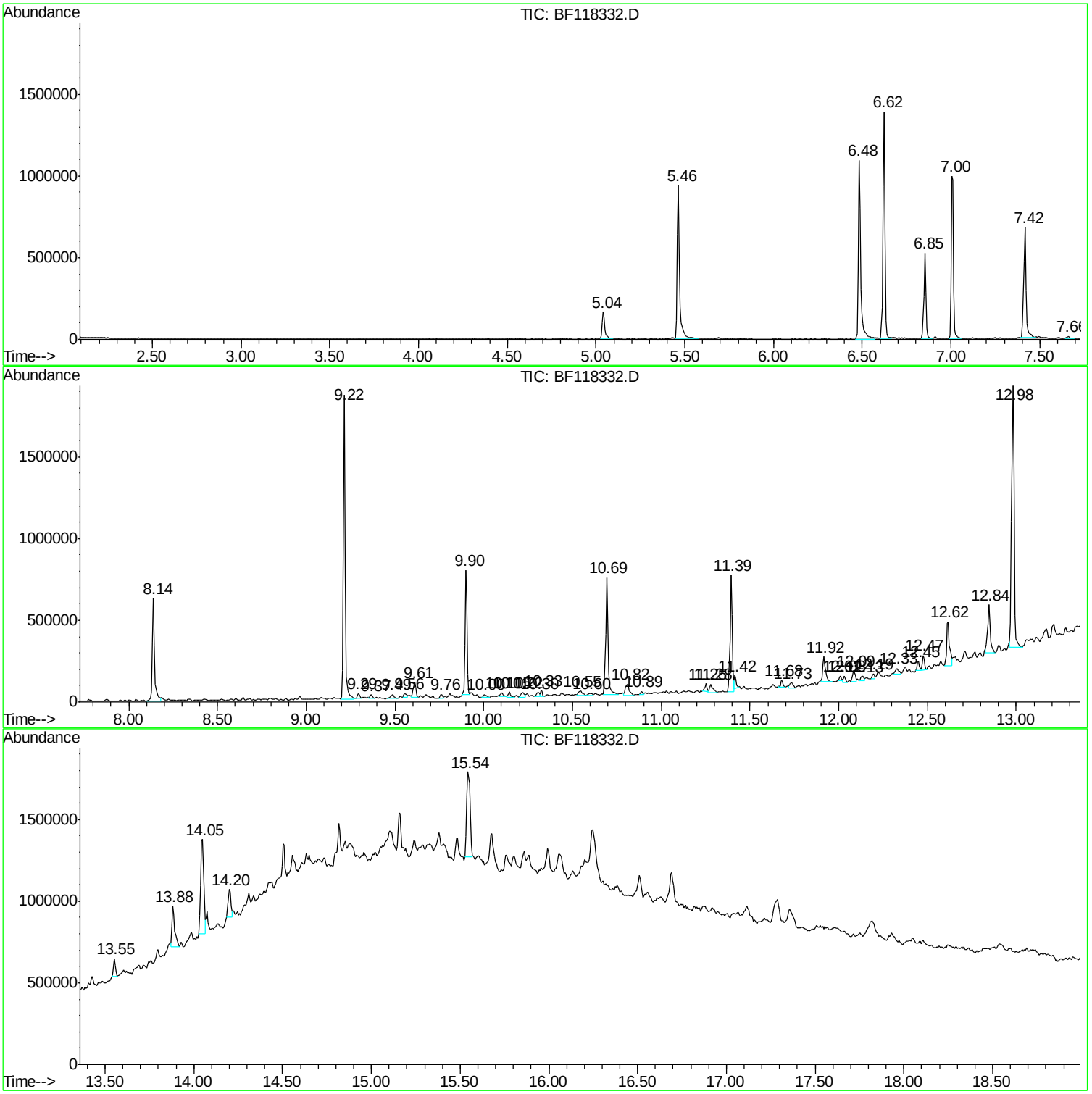
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K009-WC-2

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 : BF118332.D
Acq On : 26 Dec 2019 22:36
Operator : JU
Sample : K6436-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K009-WC-2

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

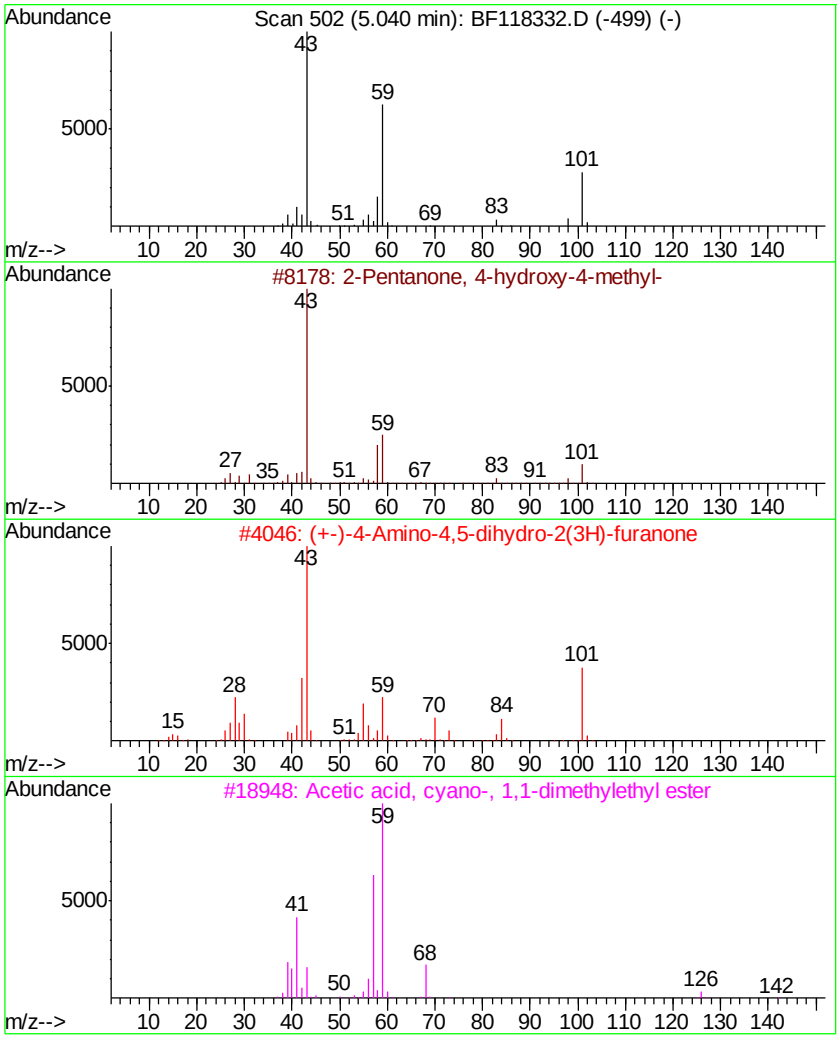
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

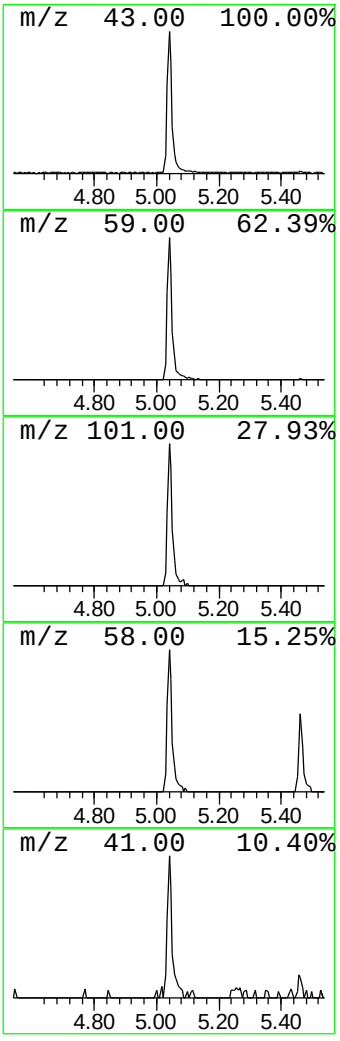
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	8.57 ng	180465	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	59
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	35
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Operator : JU
Sample : K6436-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K009-WC-2

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

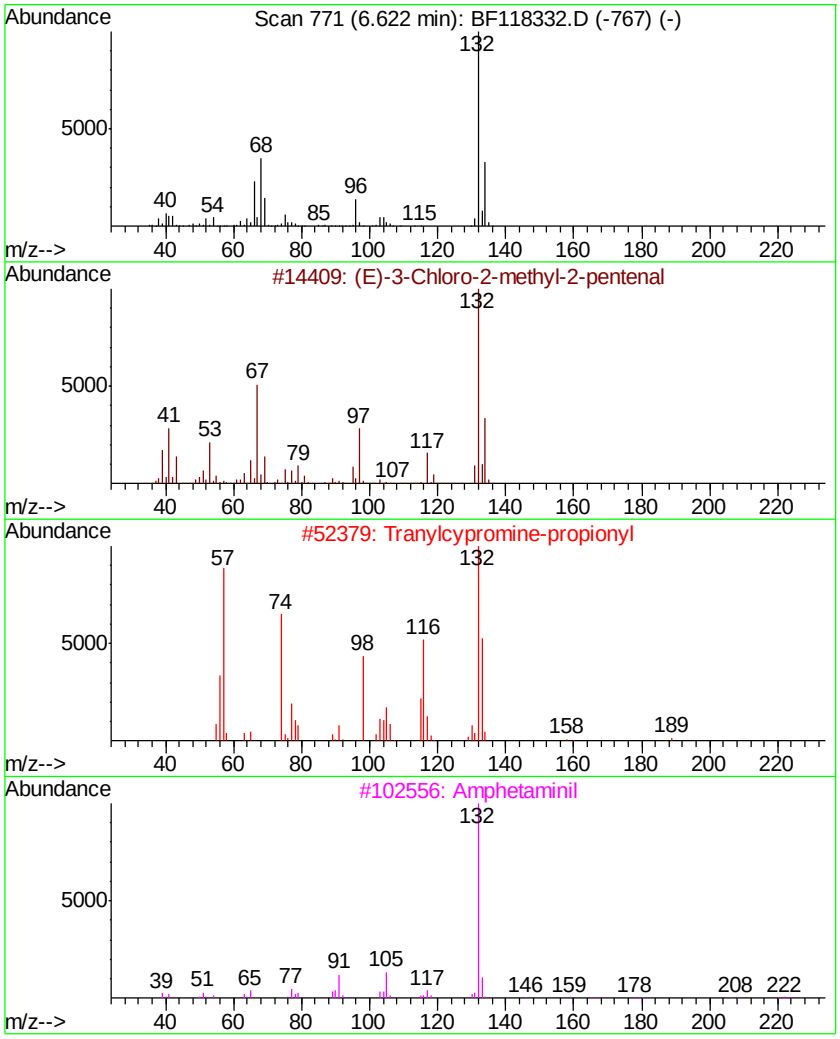
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

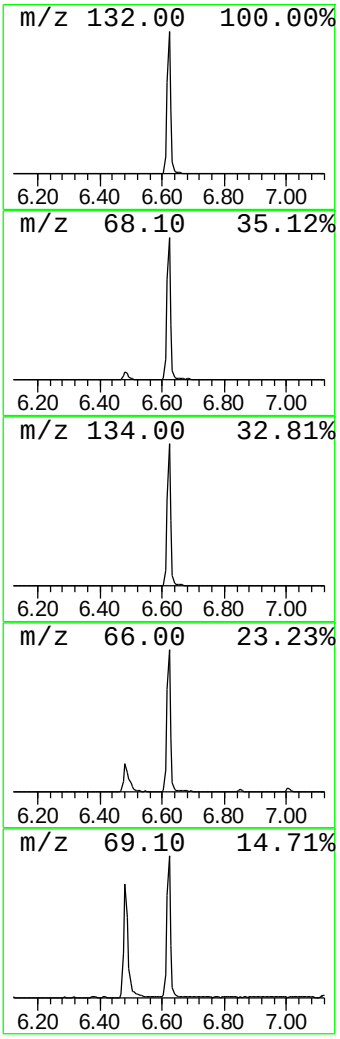
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	54.69 ng	1151780	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118332.D
Acq On : 26 Dec 2019 22:36
Operator : JU
Sample : K6436-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K009-WC-2

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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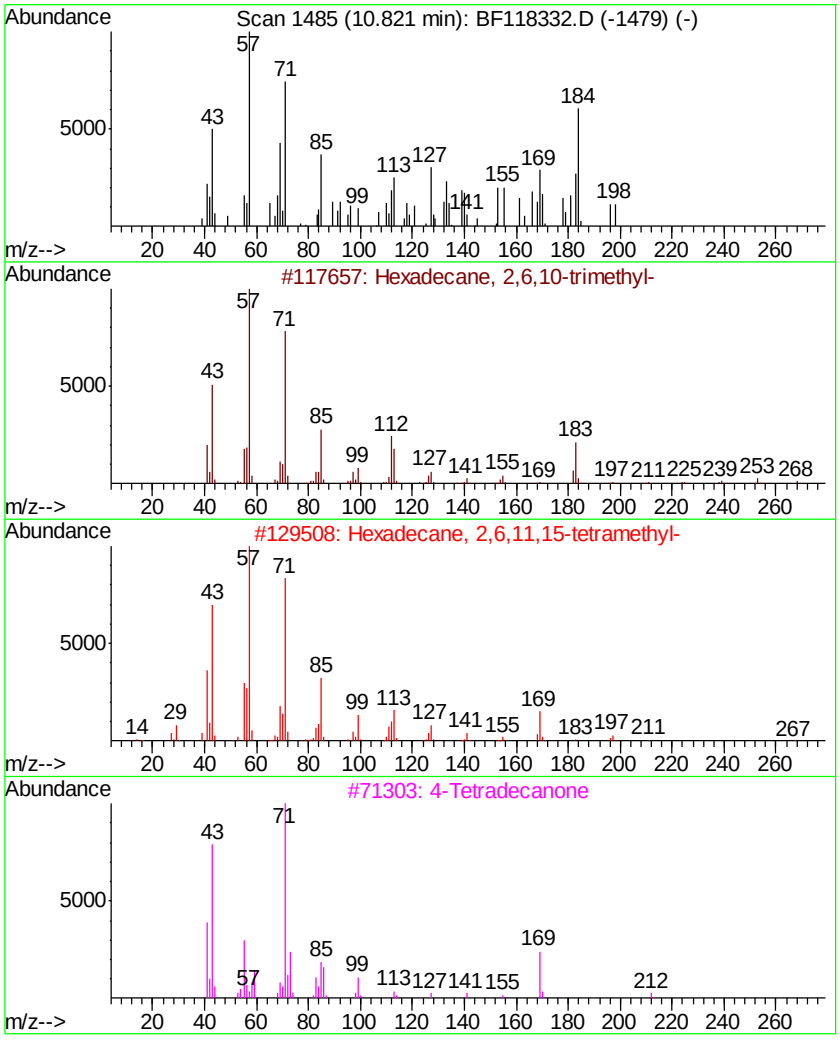
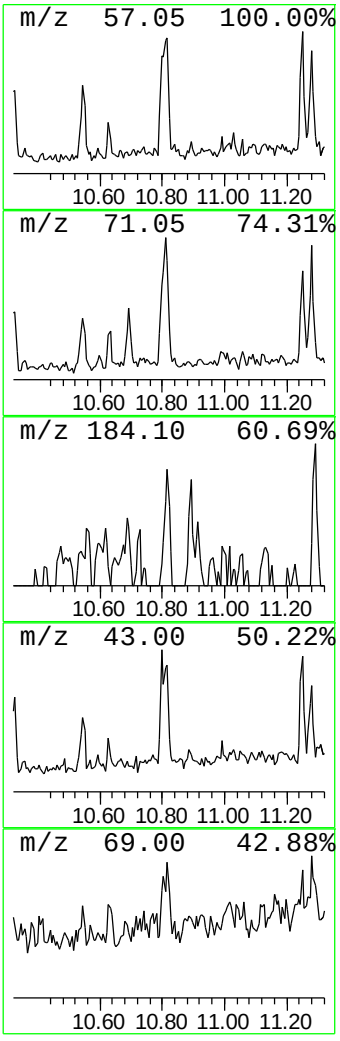
Peak Number 4 Hexadecane, 2,6,10-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.47 ng	106163	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	52
2	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	50
3	4-Tetradecanone	212	C14H28O	026496-20-8	47
4	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	46
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	46





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Sample : K6436-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K009-WC-2

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

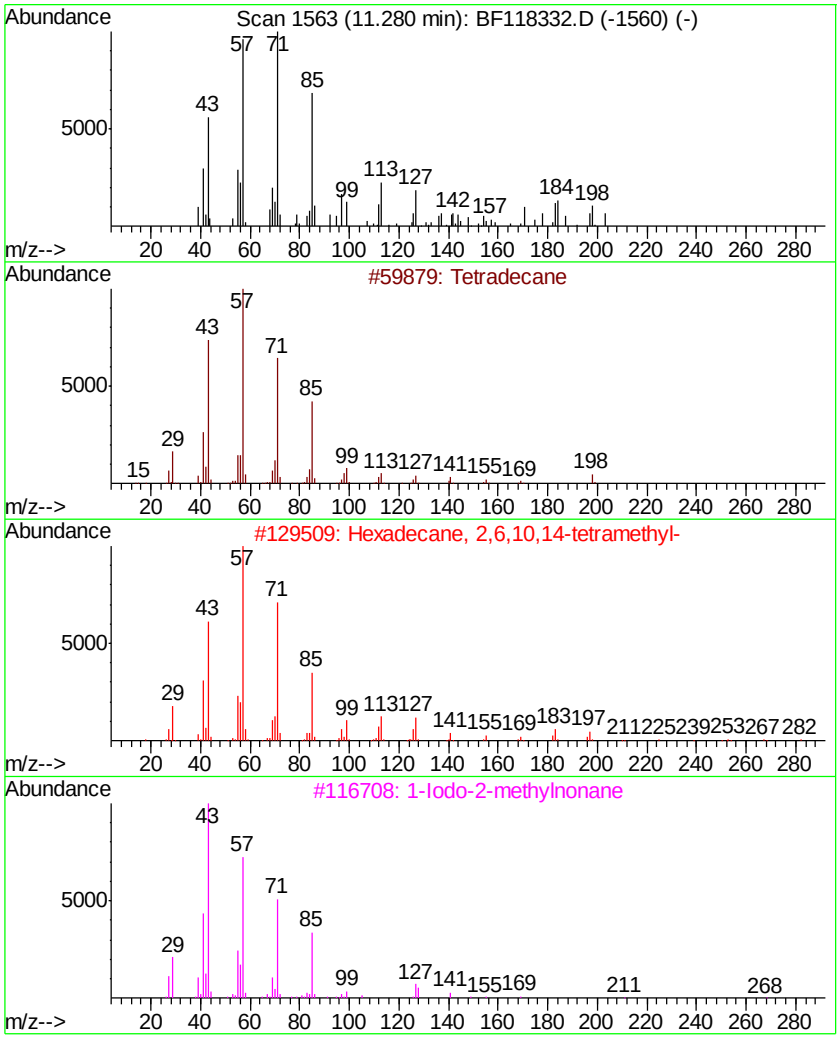
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

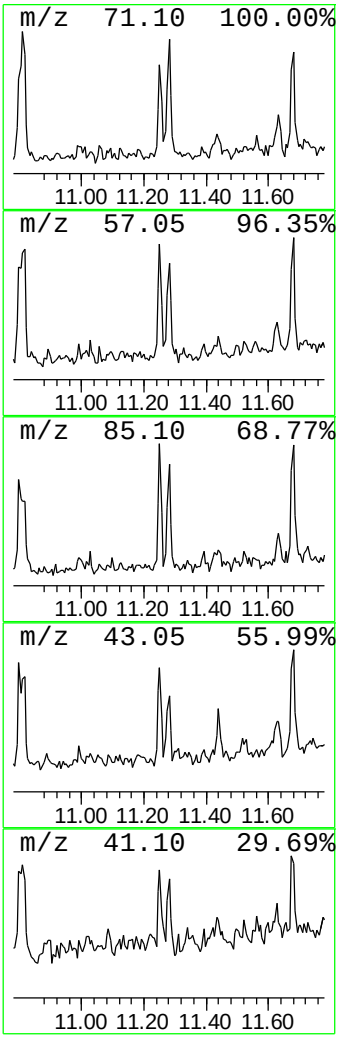
****

Peak Number 5 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.28	2.10 ng	64213	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	62
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	58
3	1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	50
4	l-Threitol, 2-O-nonyl-	248	C13H28O4	163776-15-6	47
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	43





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : K009-WC-2

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

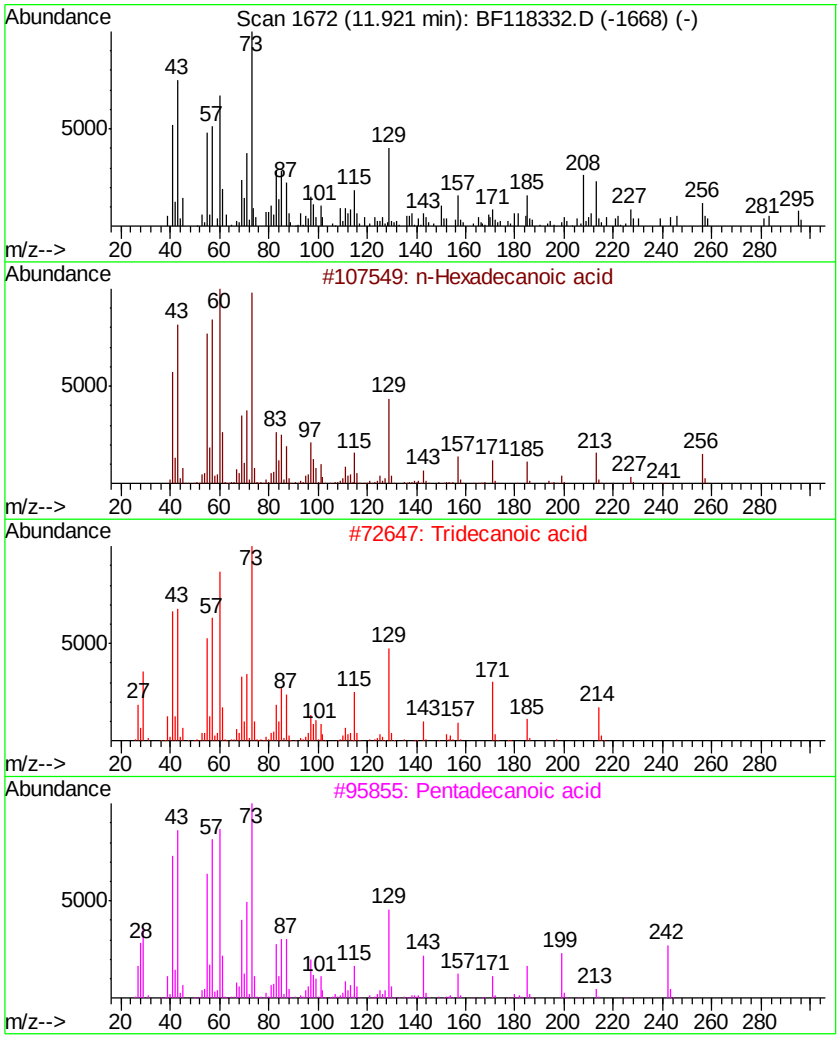
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

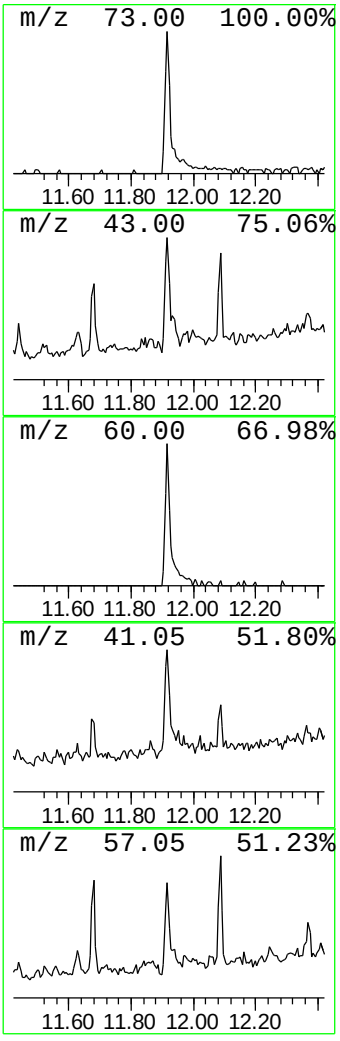
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	5.94 ng	181606	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	60
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118332.D
Acq On : 26 Dec 2019 22:36
Operator : JU
Sample : K6436-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K009-WC-2

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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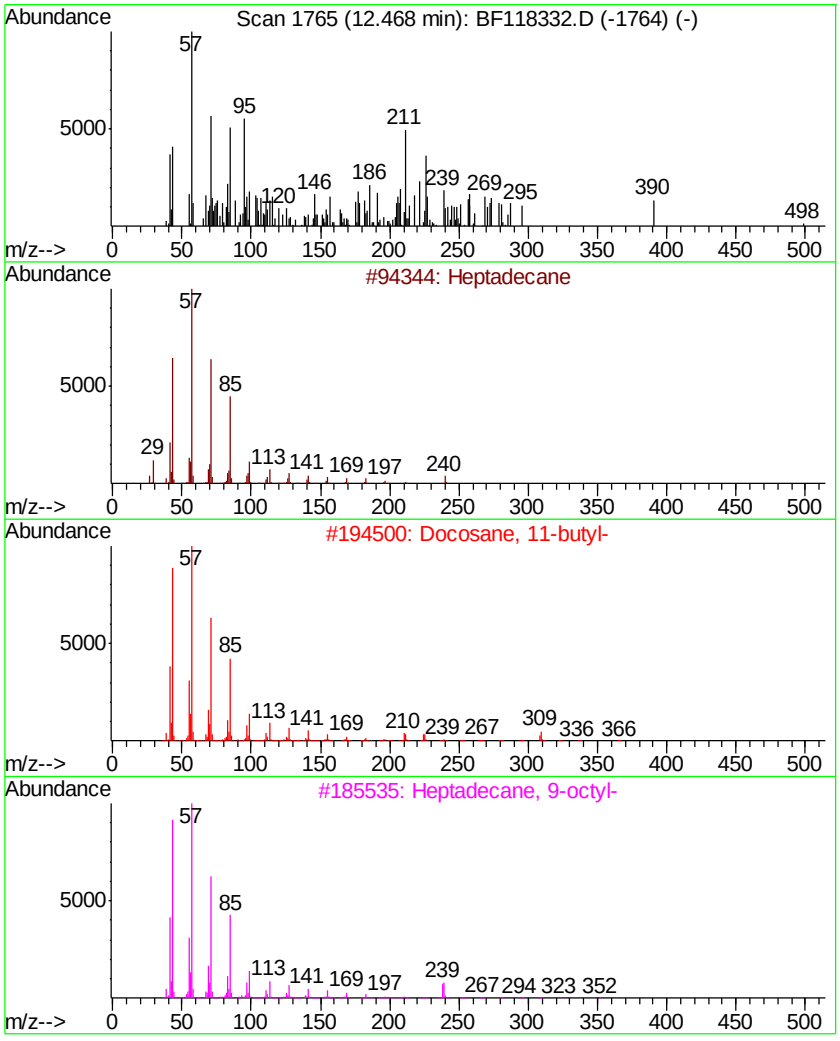
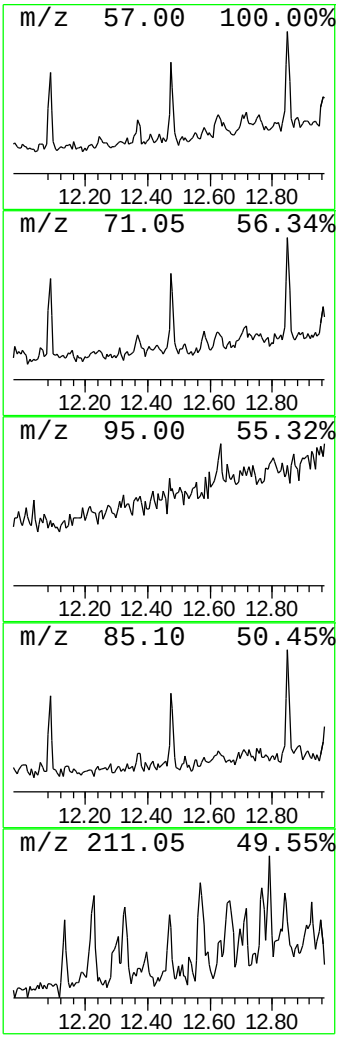
Peak Number 7 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	2.58 ng	79002	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	78
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	60
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	53
4	Hexadecane	226	C16H34	000544-76-3	53
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	53





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Misc :
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ClientSampleId : K009-WC-2

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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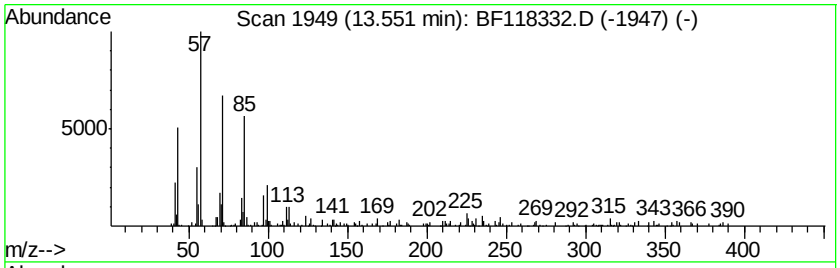
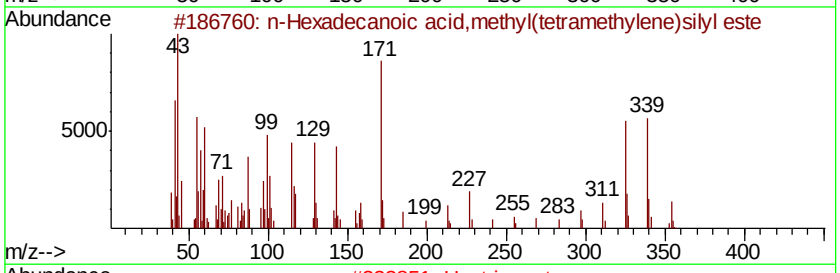
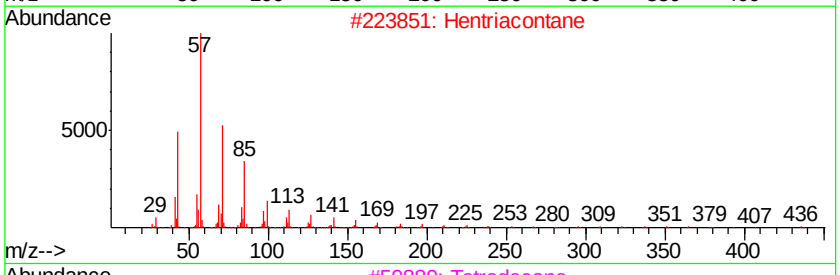
Peak Number 8 n-Hexadecanoic acid,methyl(... Concentration Rank 8

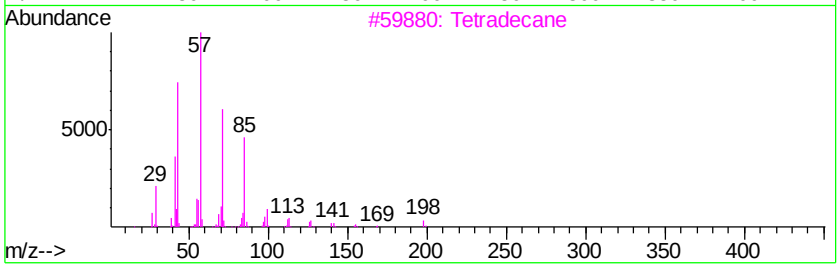
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	2.73 ng	90339	Chrysene-d12	14.05

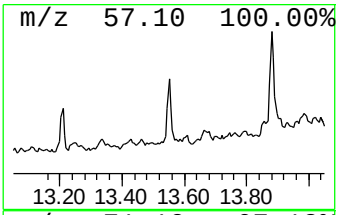
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid,methyl(tetra...	354	C21H42O2Si	1000217-04-1	90
2	Hentriacontane	437	C31H64	000630-04-6	72
3	Tetradecane	198	C14H30	000629-59-4	64
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	64
5	Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	64

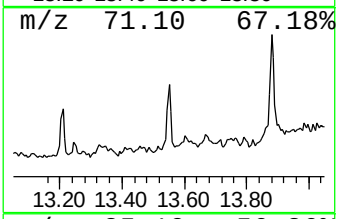


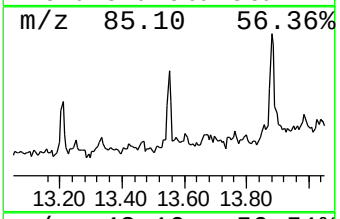


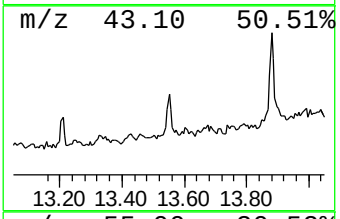


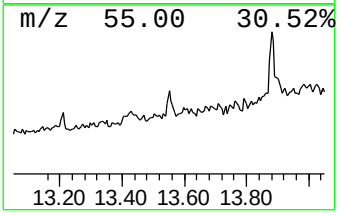












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118332.D
Acq On : 26 Dec 2019 22:36
Operator : JU
Sample : K6436-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K009-WC-2

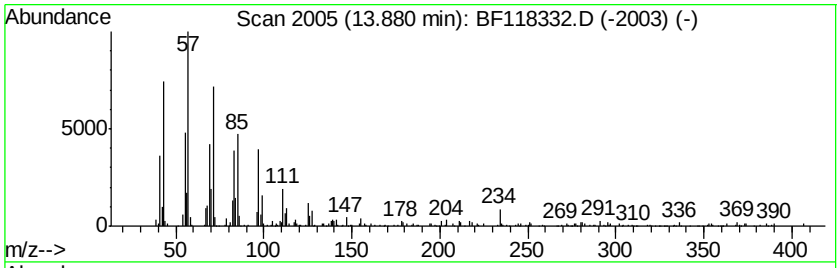
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

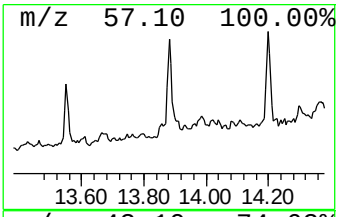
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

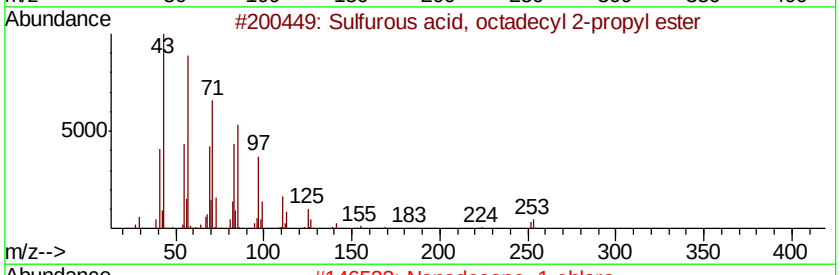
****
Peak Number 9 Sulfurous acid, octadecyl 2... Concentration Rank 3

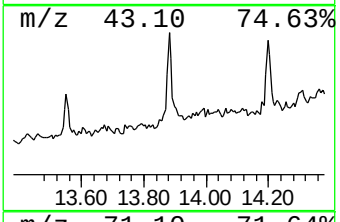
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	8.65 ng	286518	Chrysene-d12	14.05

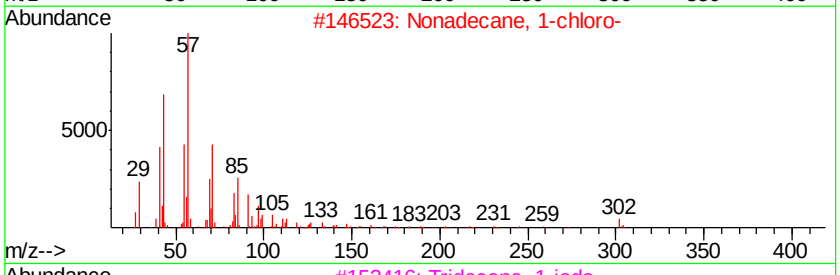
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	91
2	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	76
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
4	Pentadecane	212	C15H32	000629-62-9	62
5	Octacosanol	410	C28H58O	000557-61-9	53

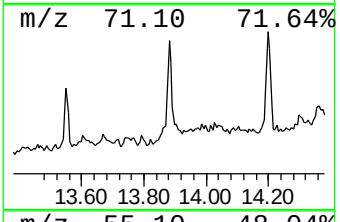


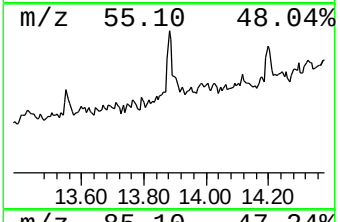


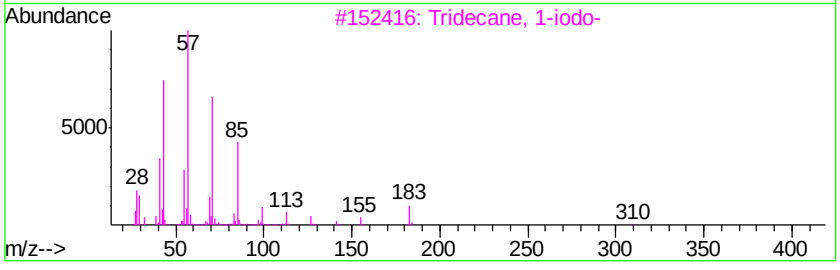


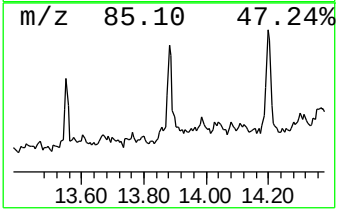












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Data File : BF118332.D
Acq On : 26 Dec 2019 22:36
Operator : JU
Sample : K6436-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K009-WC-2

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

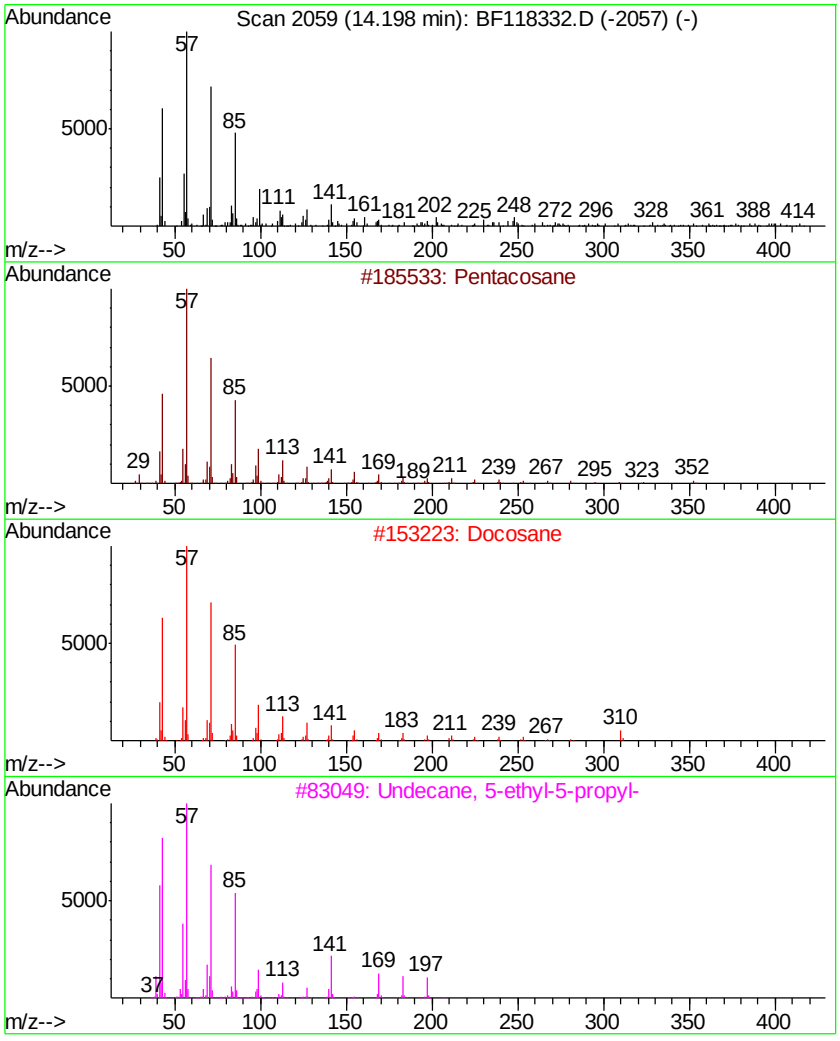
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

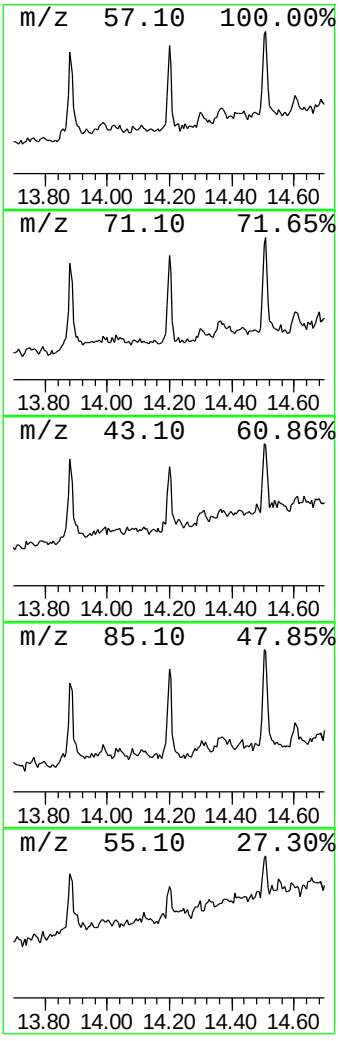
****

Peak Number 10 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	5.32 ng	176062	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	89
2	Docosane	310	C22H46	000629-97-0	80
3	Undecane, 5-ethyl-5-propyl-	226	C16H34	002755-07-9	80
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	74
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122619\
Data File : BF118332.D
Acq On : 26 Dec 2019 22:36
Operator : JU
Sample : K6436-07 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K009-WC-2

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...	5.04	8.6	ng	180465	1	6.85	421165	20.0
unknown6.62	6.62	54.7	ng	1151780	1	6.85	421165	20.0
Hexadecane, 2,6,1...	10.82	3.5	ng	106163	4	11.39	611516	20.0
Tetradecane	11.28	2.1	ng	64213	4	11.39	611516	20.0
n-Hexadecanoic acid	11.92	5.9	ng	181606	4	11.39	611516	20.0
Heptadecane	12.47	2.6	ng	79002	4	11.39	611516	20.0
n-Hexadecanoic ac...	13.55	2.7	ng	90339	5	14.05	662184	20.0
Sulfurous acid, o...	13.88	8.7	ng	286518	5	14.05	662184	20.0
Pentacosane	14.20	5.3	ng	176062	5	14.05	662184	20.0