LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 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-BF073019.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	2.140	3	9	26	rVB	940370	1229435	28.32%	3.122%
2	5.481	572	577	580	rBV	3636197	3821416	88.02%	9.703%
3	6.492	743	749	752	rBV	3603238	4037215	92.99%	10.251%
4	6.628	767	772	775	rBV	4059334	4095579	94.33%	10.399%
5	6.851	806	810	818	rBV	1215325	974267	22.44%	2.474%
6	7.010	833	837	840	rBV	3589142	3222500	74.22%	8.182%
7	7.416	901	906	909	rBV	2690807	2641417	60.84%	6.707%
8	8.133	1024	1028	1046	rBV	1310858	1198476	27.60%	3.043%
9	9.216	1207	1212	1215	rBV	4493497	4341548	100.00%	11.024%
10	9.604	1274	1278	1296	rBV	436430	395208	9.10%	1.003%
11	9.892	1323	1327	1343	rBV	1579436	1349252	31.08%	3.426%
12	10.680	1457	1461	1478	rBV	2310935	2505470	57.71%	6.362%
13	11.380	1576	1580	1583	rBV	1293444	1173576	27.03%	2.980%
14	11.904	1667	1669	1677	rBV3	125775	141458	3.26%	0.359%
15	12.592	1783	1786	1791	rBV	105554	96028	2.21%	0.244%
16	12.692	1800	1803	1810	rBV2	31305	48389	1.11%	0.123%
17	12.821	1821	1825	1830	rVB	107630	110789	2.55%	0.281%
18	12.962	1845	1849	1853	rBV	3478163	3465125	79.81%	8.799%
19	13.439	1923	1930	1940	rBV	848744	831483	19.15%	2.111%
20	13.886	1997	2006	2020	rBV6	74791	245851	5.66%	0.624%
21	14.021	2022	2029	2032	rVV	1076592	1065061	24.53%	2.704%
22	14.045	2032	2033	2040	rVB	71405	51612	1.19%	0.131%
23	14.180	2052	2056	2058	rBV	54206	51837	1.19%	0.132%
24	14.480	2103	2107	2111	rBV	115037	118670	2.73%	0.301%
25	14.786	2156	2159	2164	rVB	171598	159967	3.68%	0.406%
26	15.062	2202	2206	2209	rBV	56907	82876	1.91%	0.210%
27	15.121	2213	2216	2221	rVB	177288	205801	4.74%	0.523%
28	15.362	2254	2257	2261	rVB	39534	44620	1.03%	0.113%
29	15.427	2264	2268	2273	rVB	51021	70208	1.62%	0.178%
30	15.492	2273	2279	2288	rBV	826395	1212281	27.92%	3.078%
31	15.939	2349	2355	2362	rBV	136105	214747	4.95%	0.545%
32	16.439	2435	2440	2452	rBV3	79417	180940	4.17%	0.459%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 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-BF073019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

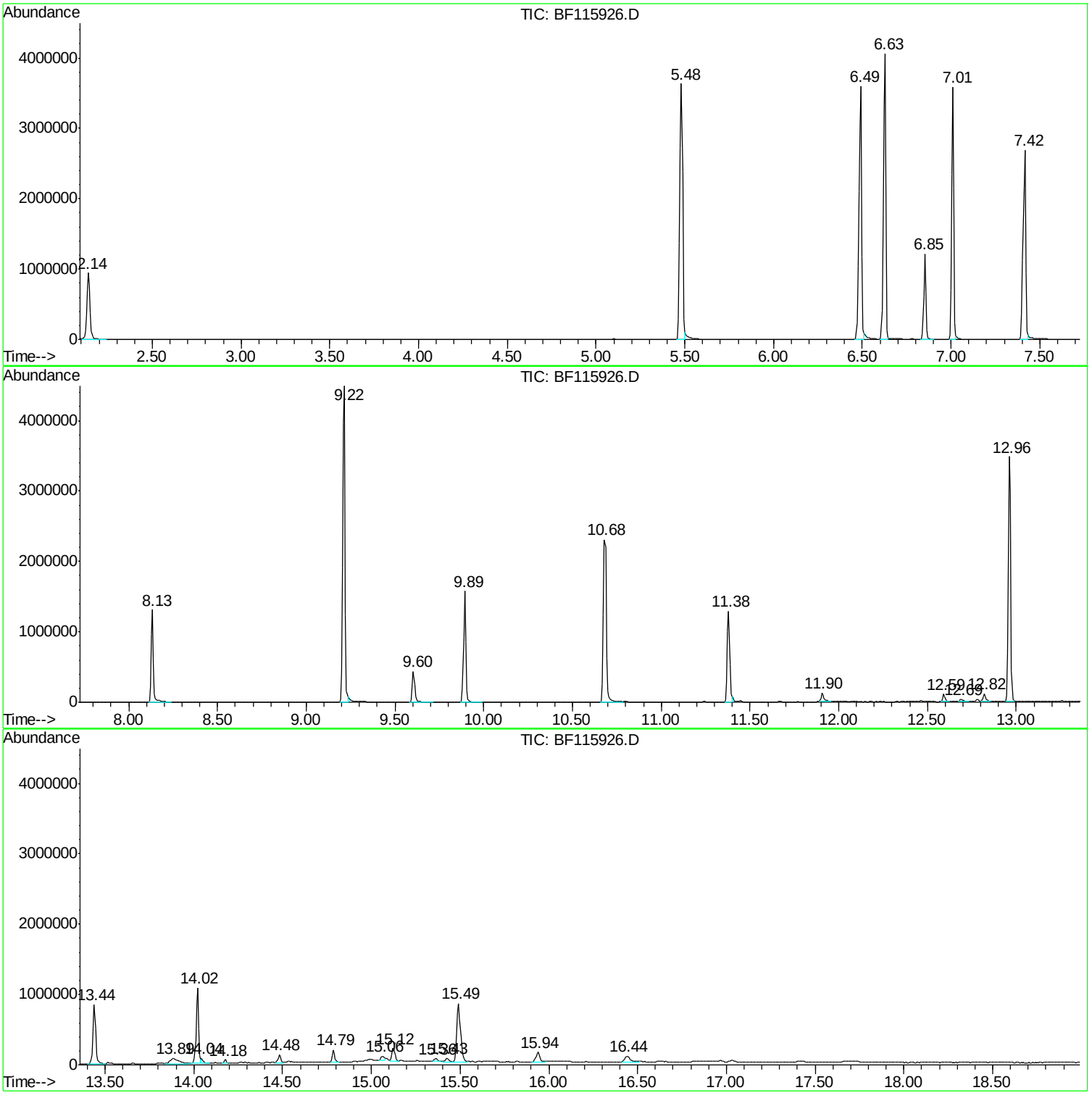
Sum of corrected areas: 39383102

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

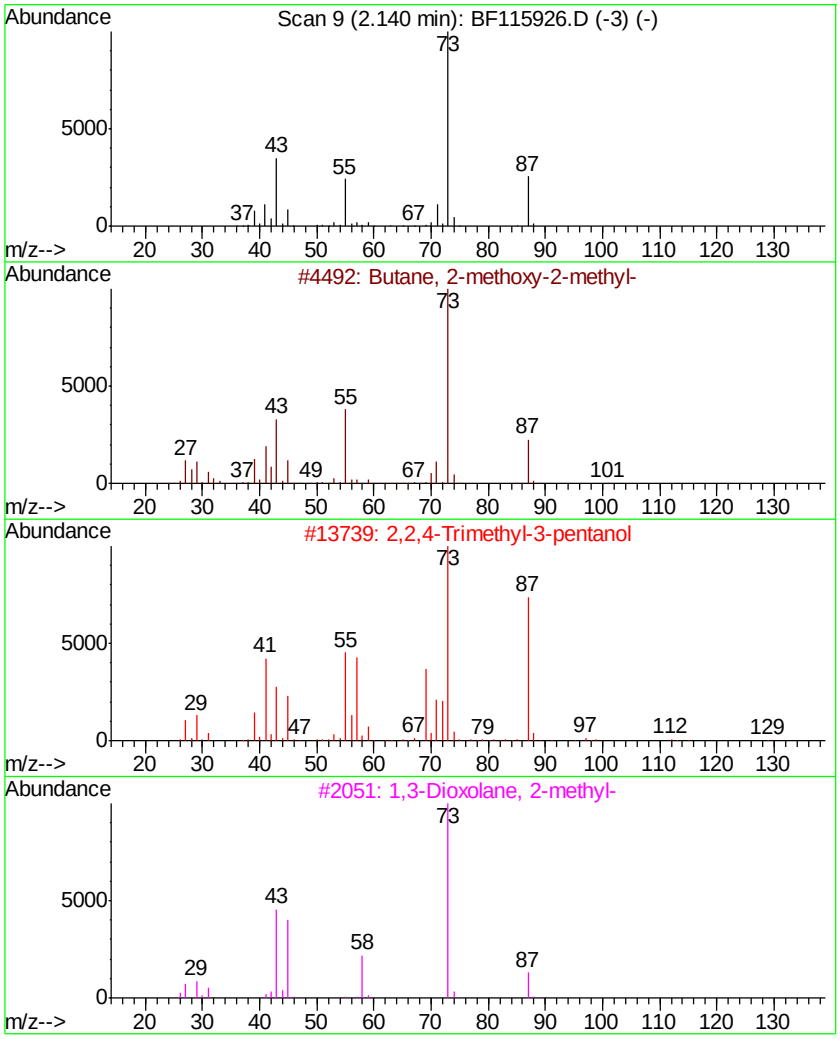
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

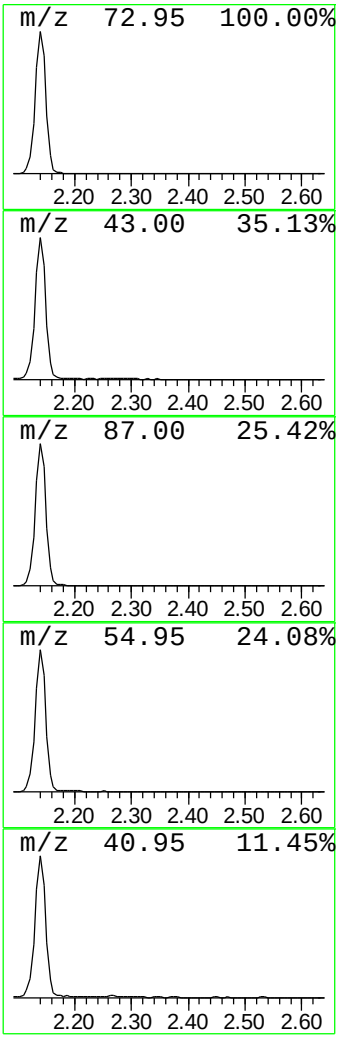
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	25.24 ng	1229440	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

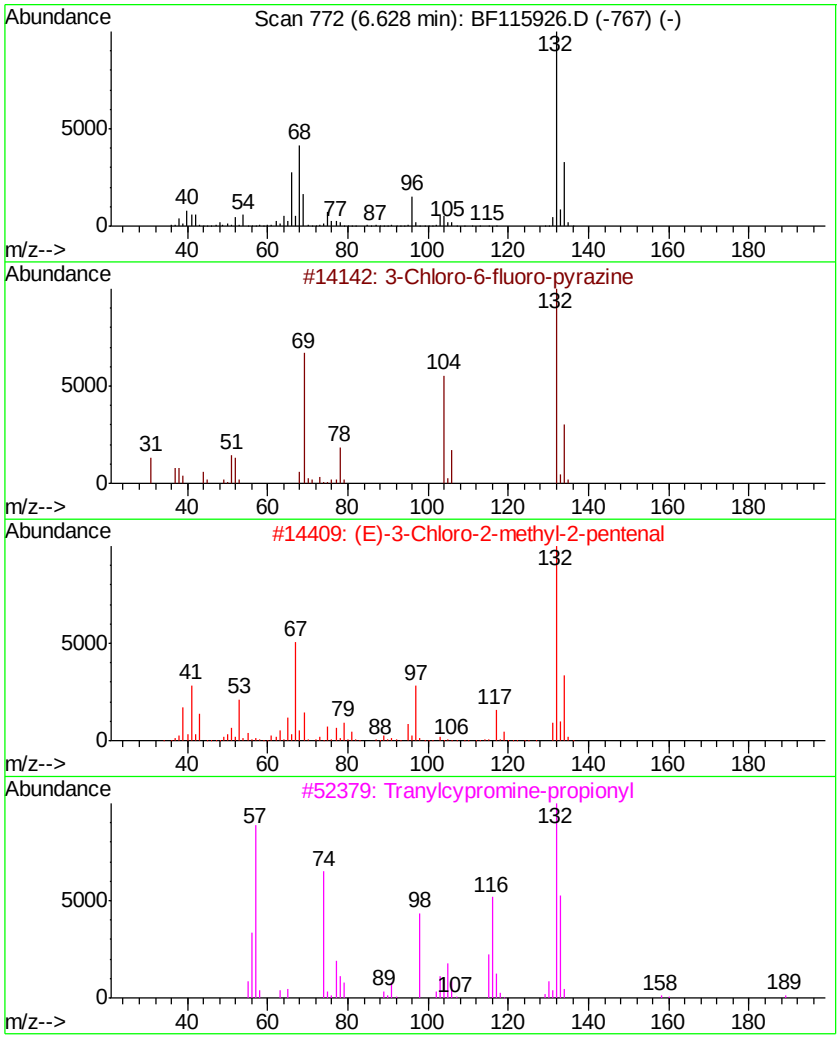
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

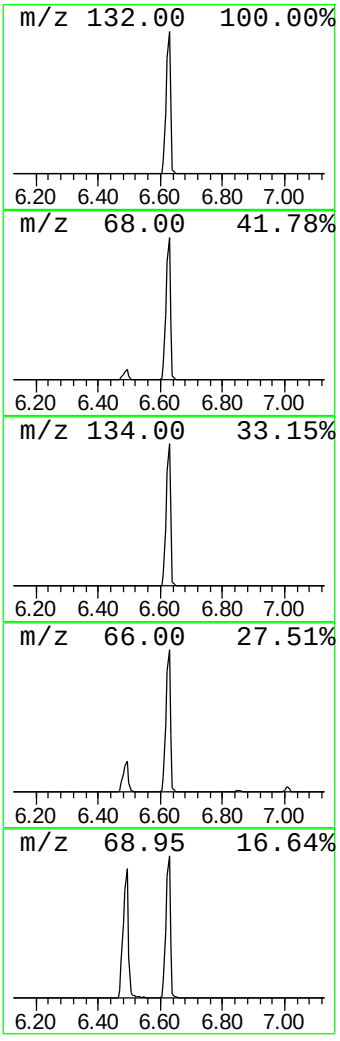
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	84.08 ng	4095580	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	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	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\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

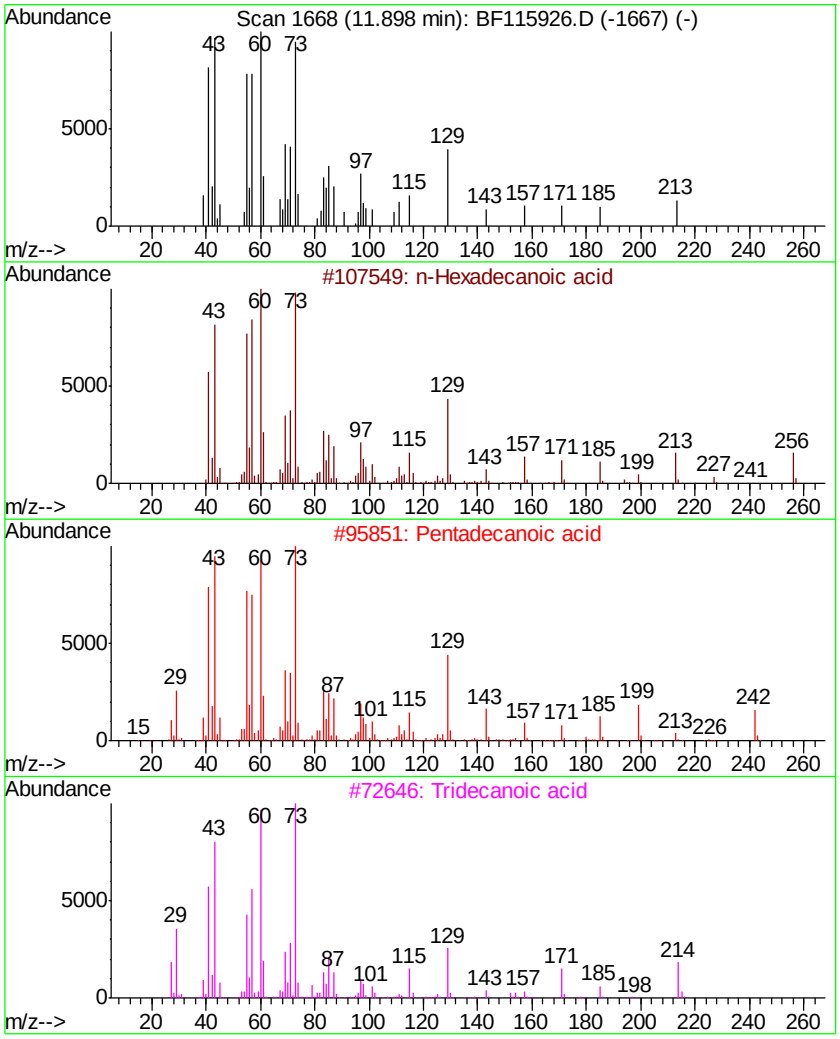
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

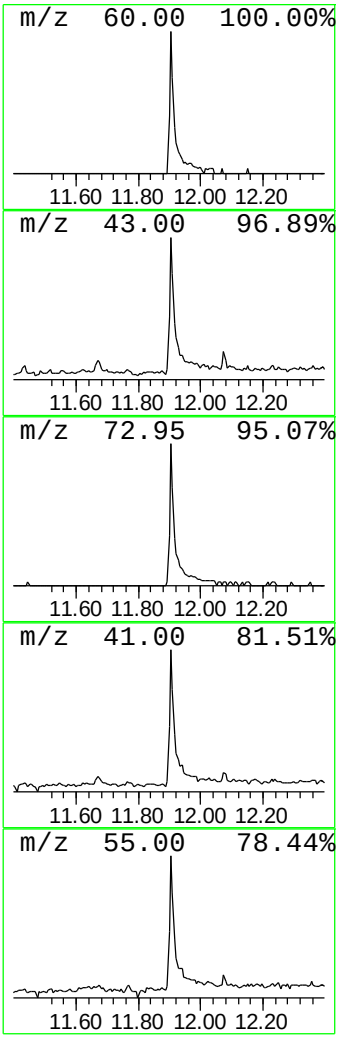
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.41 ng	141458	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	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

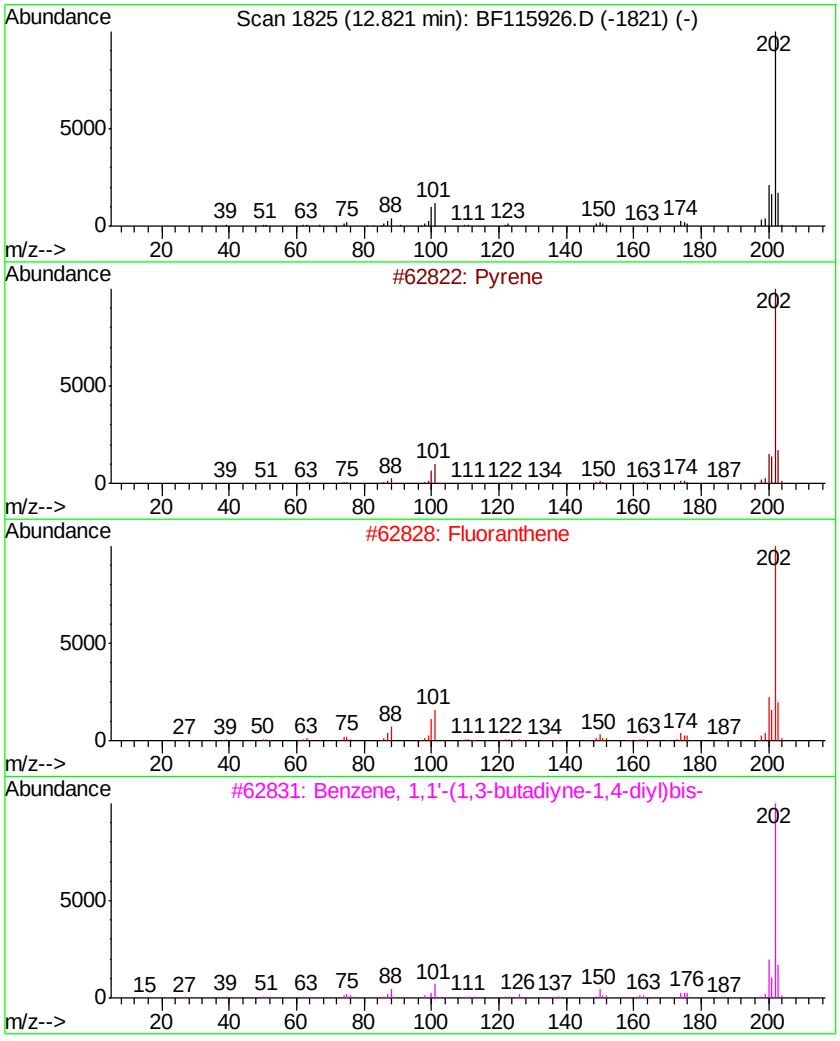
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

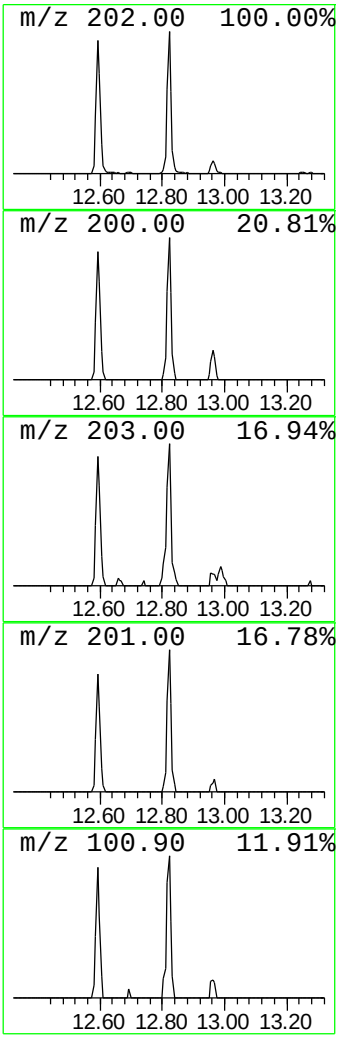
****

Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	2.08 ng	110789	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	93
2	Fluoranthene	202	C16H10	000206-44-0	91
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	59
4	Pyrimidine, 4-methoxy-6-(2-hydro...	202	C11H10N2O2	097630-79-0	40
5	Succinic acid, 4-cyanophenyl 2,3...	363	C17H11Cl2NO4	1000360-70-9	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

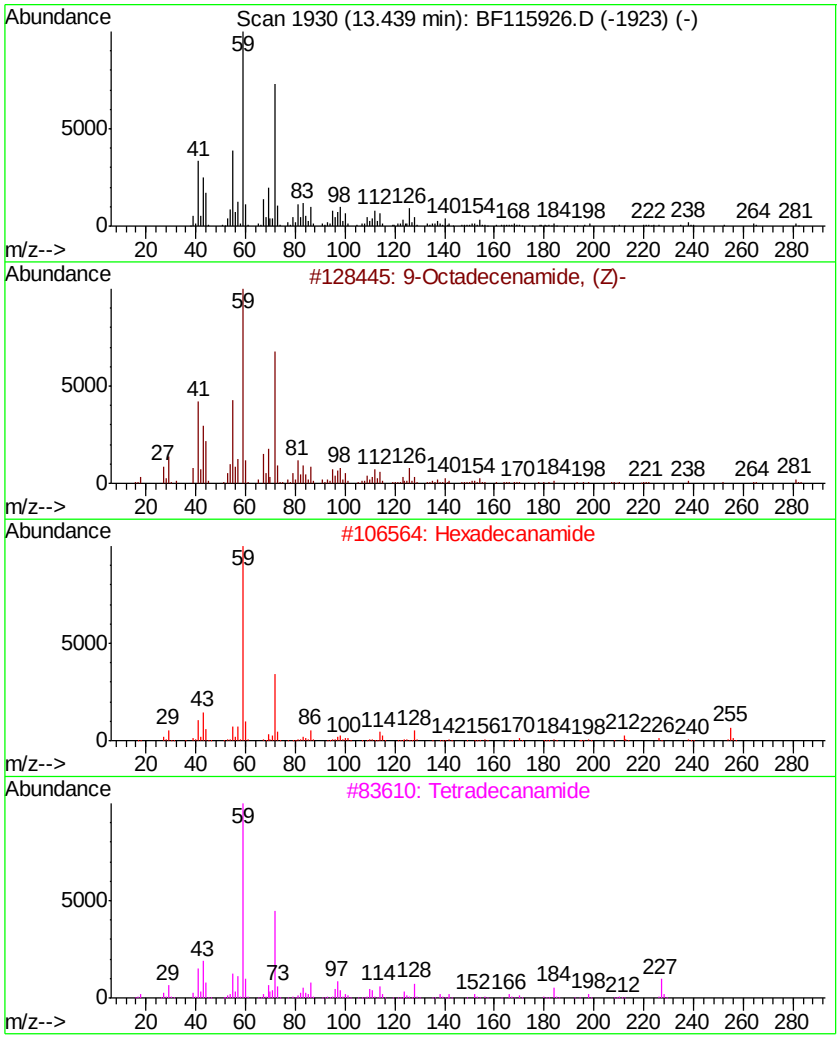
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

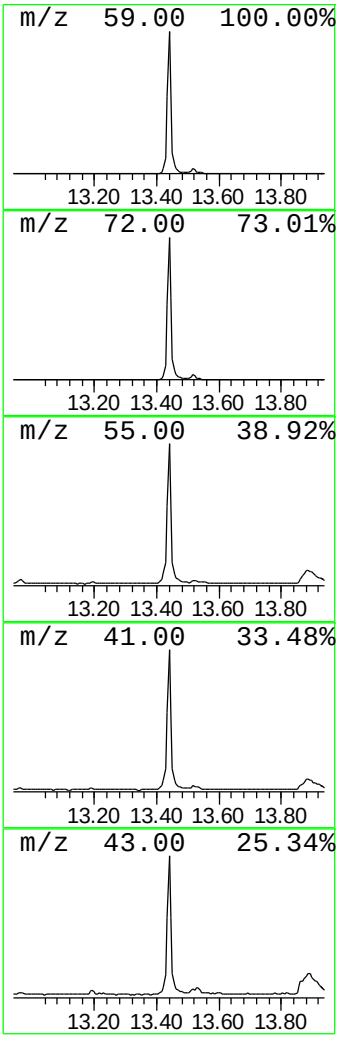
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	15.61 ng	831483	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Hexadecanamide	255	C16H33NO	000629-54-9	72
3	Tetradecanamide	227	C14H29NO	000638-58-4	72
4	Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	59
5	Dodecanamide	199	C12H25NO	001120-16-7	59





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Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

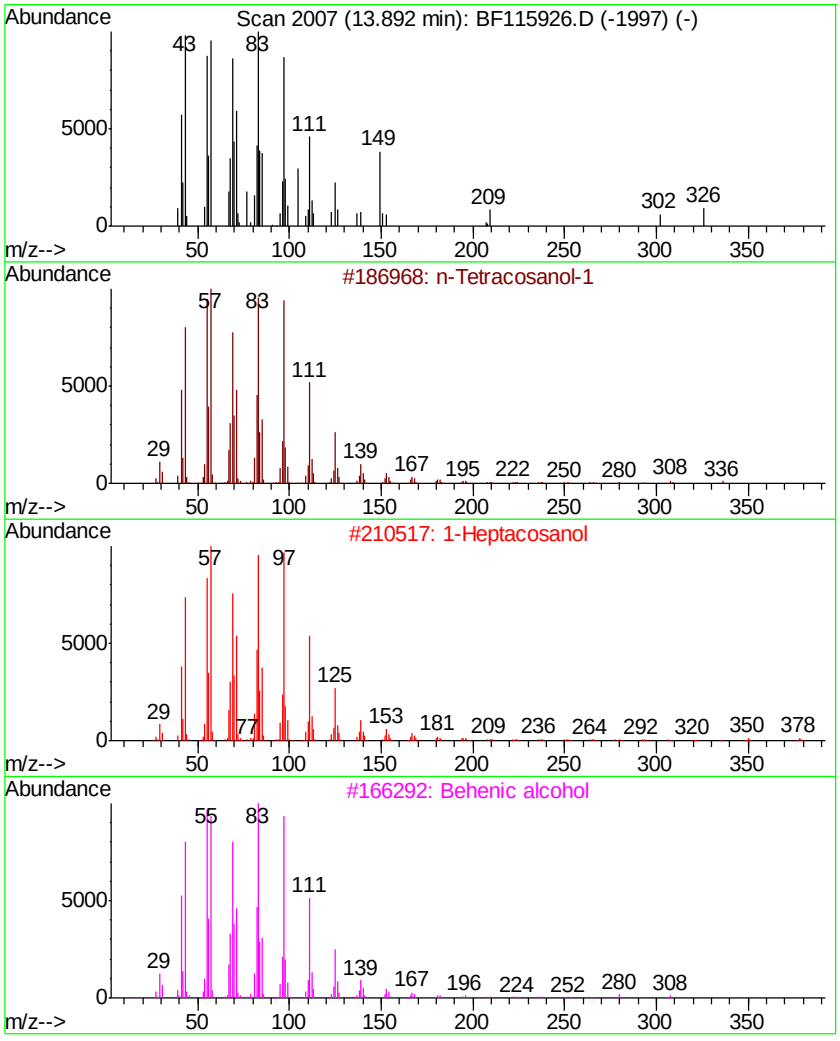
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

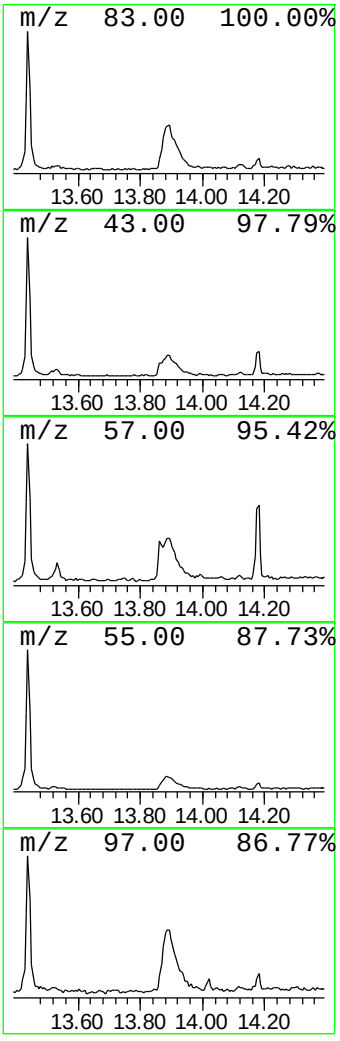
****

Peak Number 7 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	4.62 ng	245851	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	1-Heptacosanol	396	C27H56O	002004-39-9	93
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
5	Octacosyl acetate	452	C30H60O2	018206-97-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

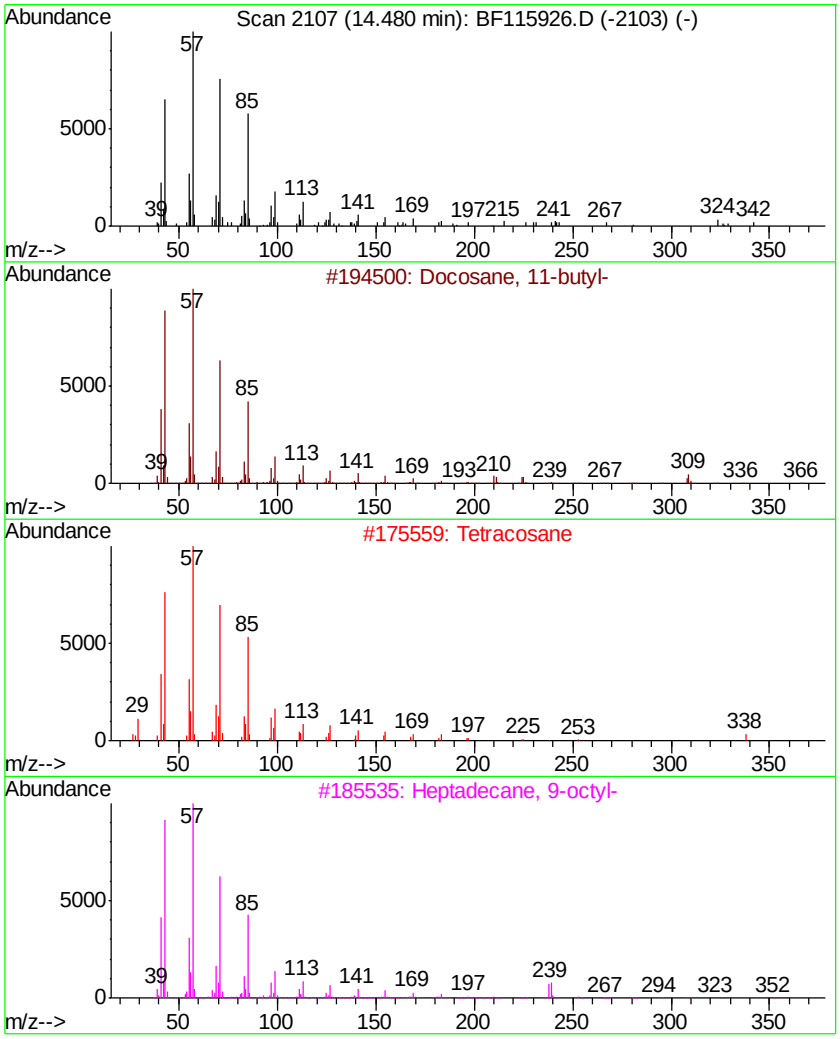
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

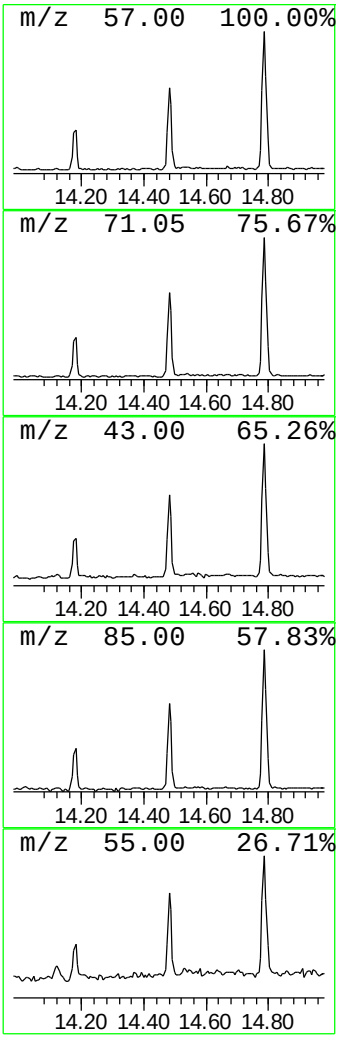
****

Peak Number 8 Docosane, 11-butyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	2.23 ng	118670	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

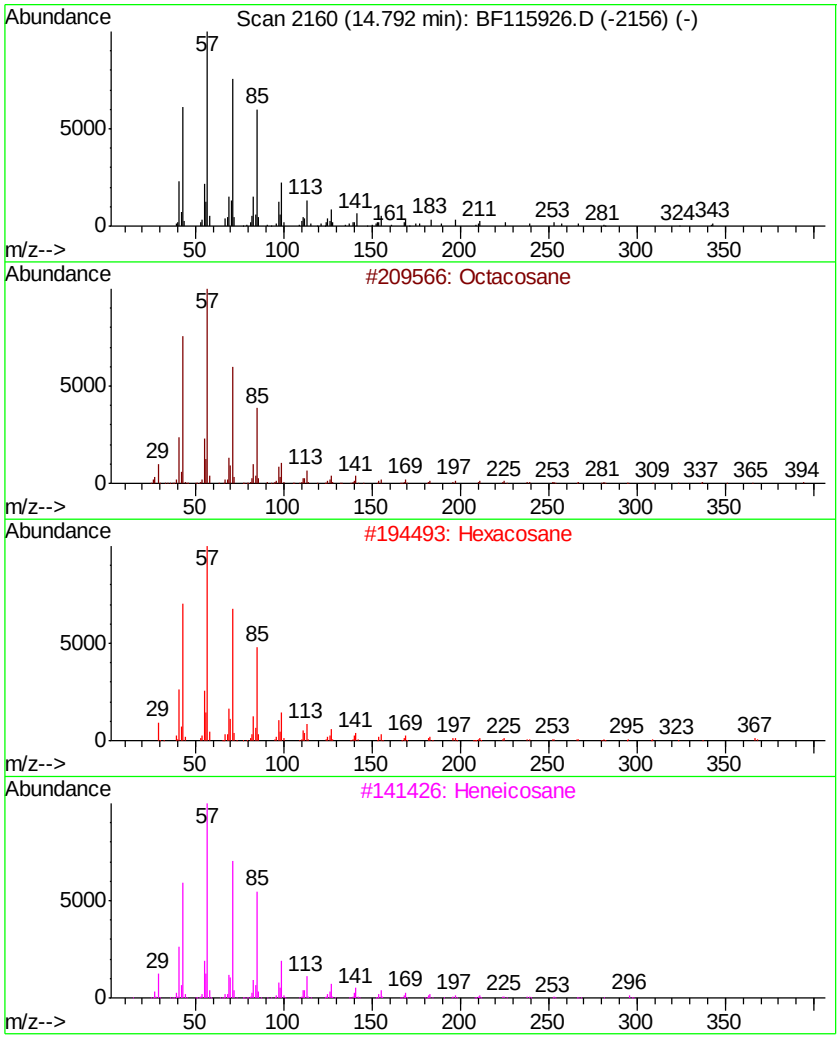
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

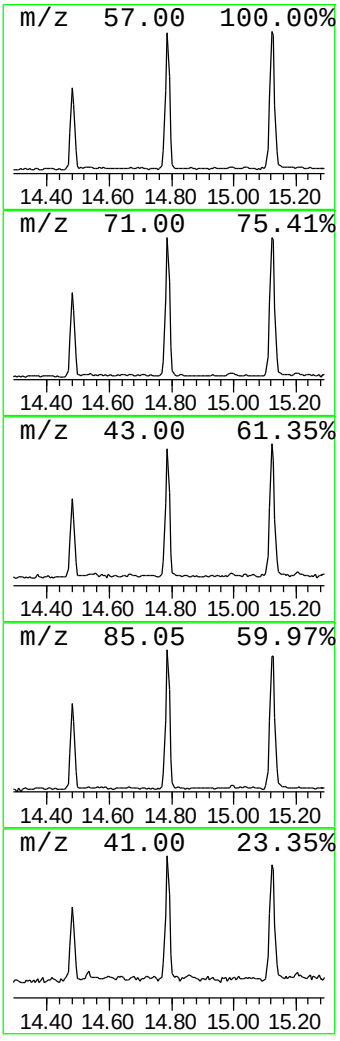
****

Peak Number 9 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.64 ng	159967	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

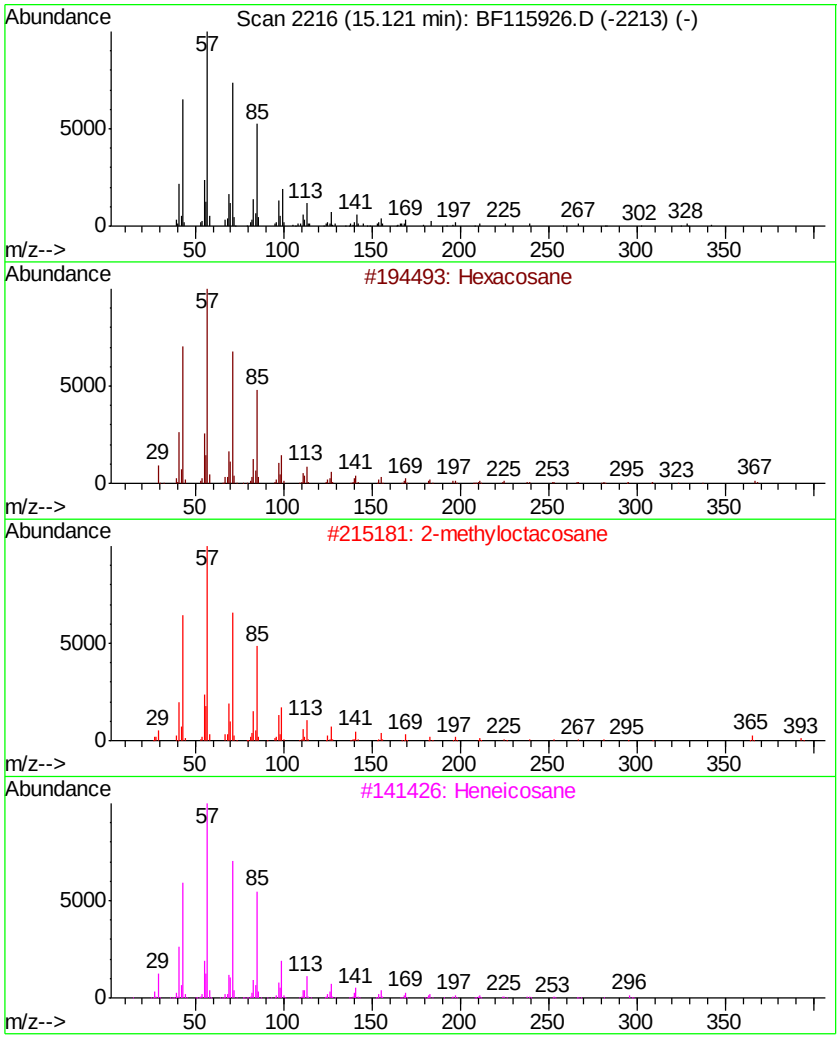
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

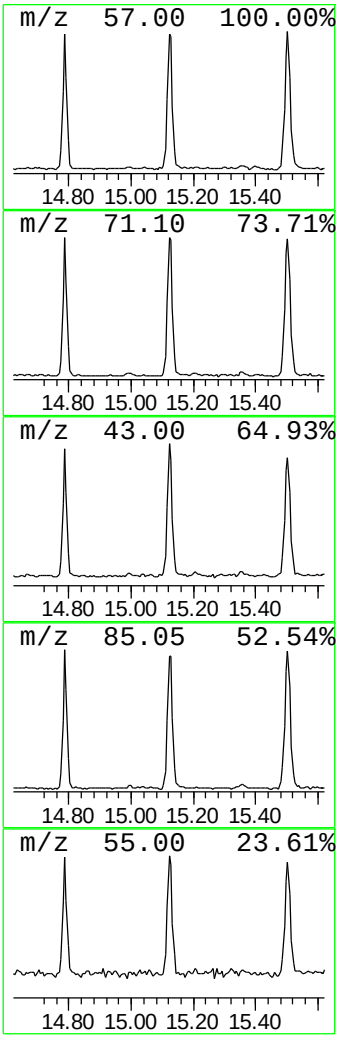
****

Peak Number 10 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	3.40 ng	205801	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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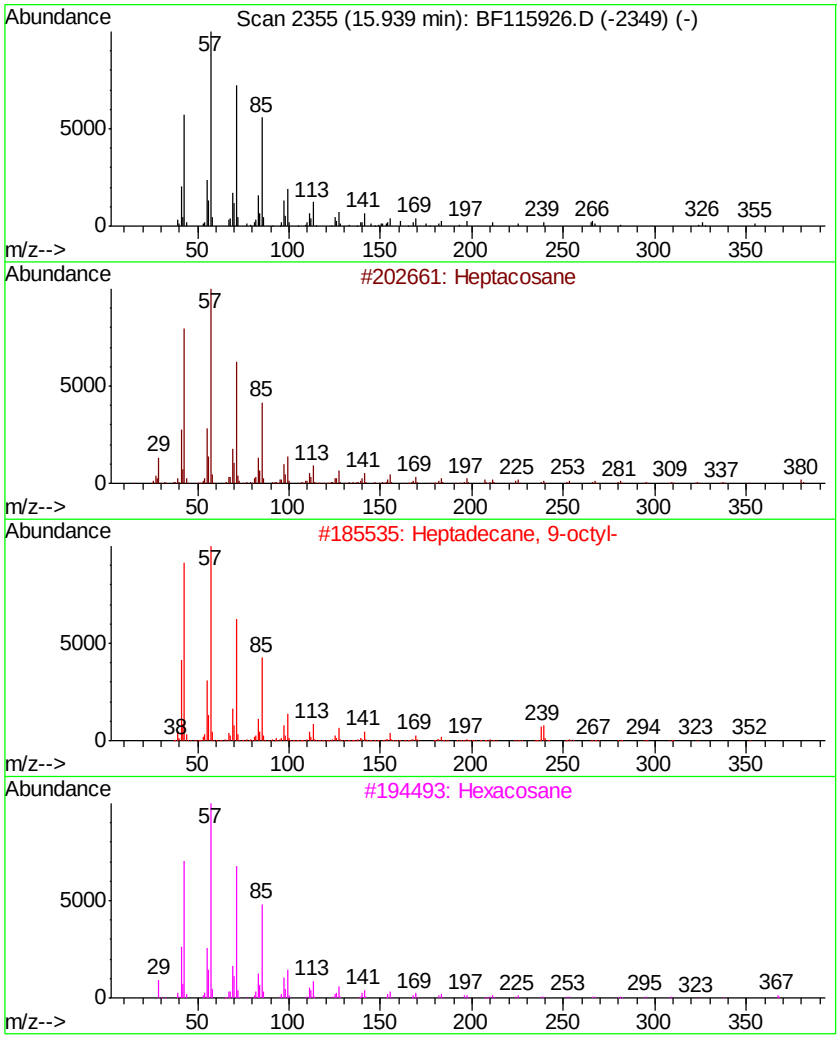
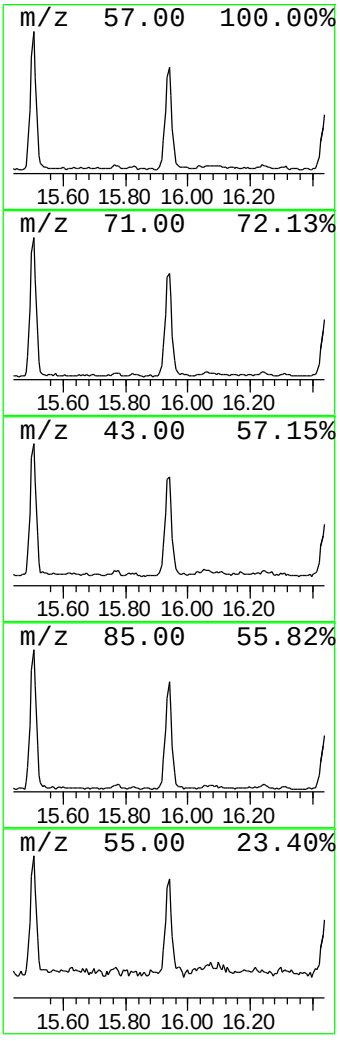
Peak Number 11 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	3.54 ng	214747	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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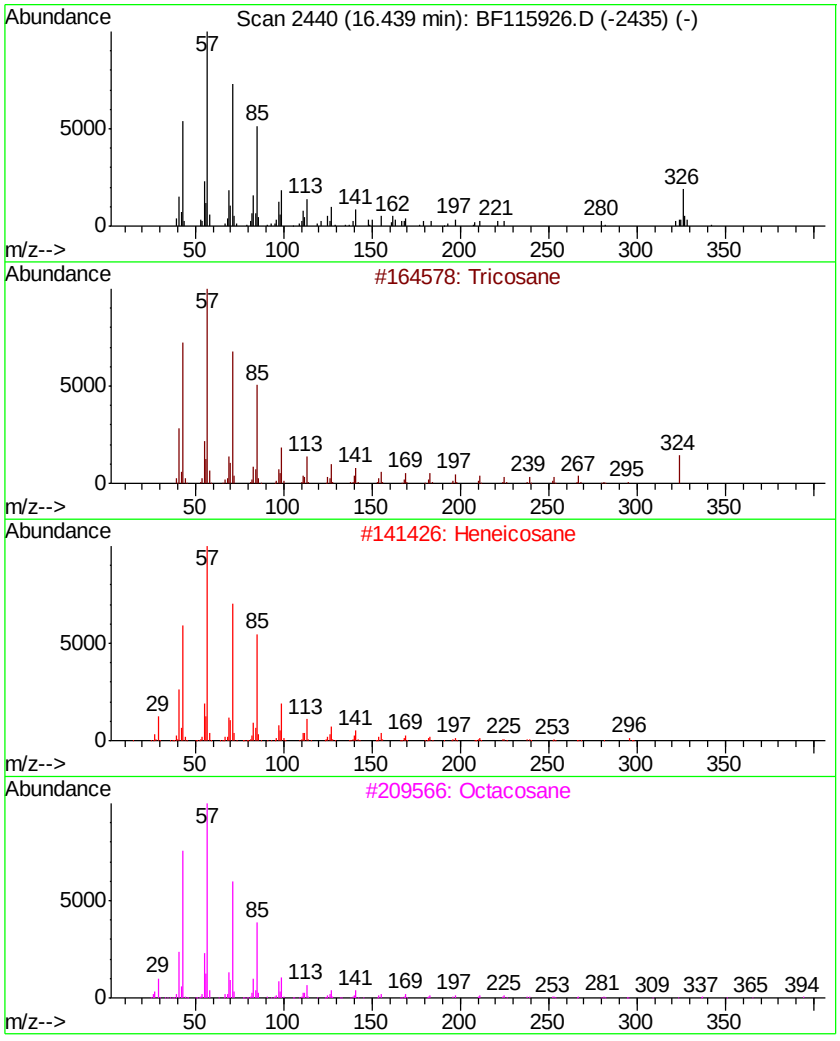
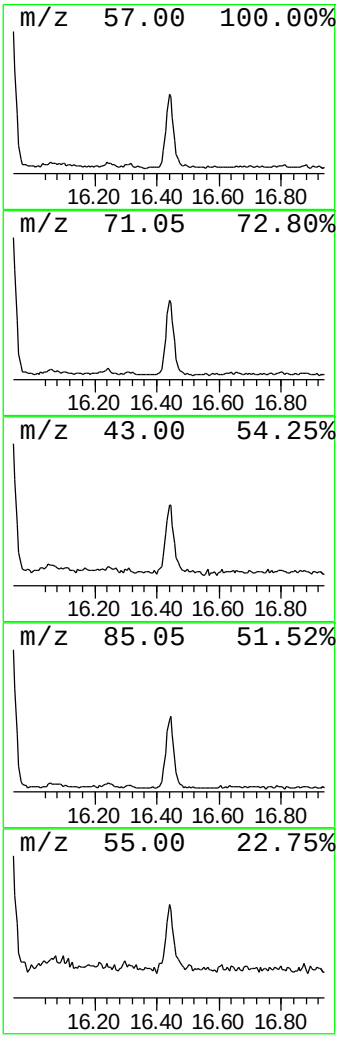
Peak Number 12 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	2.99 ng	180940	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	91
2	Heneicosane	296	C21H44	000629-94-7	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Docosane, 11-decyl-	451	C32H66	055401-55-3	87
5	Hentriacontane	437	C31H64	000630-04-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080119\
Data File : BF115926.D
Acq On : 2 Aug 2019 00:09
Operator : HP/JU
Sample : K4044-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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...	2.14	25.2	ng	1229440	1	6.85	974267	20.0
unknown6.63	6.63	84.1	ng	4095580	1	6.85	974267	20.0
n-Hexadecanoic acid	11.90	2.4	ng	141458	4	11.38	1173580	20.0
Benzene, 1,1'-(1,...	12.82	2.1	ng	110789	5	14.02	1065060	20.0
9-Octadecenamide,...	13.44	15.6	ng	831483	5	14.02	1065060	20.0
n-Tetracosanol-1	13.89	4.6	ng	245851	5	14.02	1065060	20.0
Docosane, 11-butyl-	14.48	2.2	ng	118670	5	14.02	1065060	20.0
Octacosane	14.79	2.6	ng	159967	6	15.49	1212280	20.0
Hexacosane	15.12	3.4	ng	205801	6	15.49	1212280	20.0
Heptacosane	15.94	3.5	ng	214747	6	15.49	1212280	20.0
Tricosane	16.44	3.0	ng	180940	6	15.49	1212280	20.0