LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110646.D
Acq On : 9 Nov 2018 23:52
Operator : JU/SJ
Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

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-BF110818.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	2.275	27	32	43	rVB	94717	131881	4.84%	0.611%
2	5.198	525	529	547	rBV	70651	110099	4.04%	0.510%
3	5.569	587	592	613	rBV	2161805	2421926	88.92%	11.222%
4	6.575	758	763	778	rBV	2166563	2723800	100.00%	12.620%
5	6.716	782	787	790	rBV	2585337	2569943	94.35%	11.908%
6	6.945	822	826	832	rBV	584366	483572	17.75%	2.241%
7	7.104	848	853	856	rBV	1976688	1897327	69.66%	8.791%
8	7.510	917	922	933	rBV	1443886	1631280	59.89%	7.558%
9	8.228	1040	1044	1049	rBV	689093	621444	22.82%	2.879%
10	8.875	1152	1154	1159	rVB2	26081	30695	1.13%	0.142%
11	9.298	1221	1226	1230	rBV	2552251	2517466	92.42%	11.664%
12	9.692	1287	1293	1299	rVB	193378	215518	7.91%	0.999%
13	9.986	1339	1343	1346	rBV	740397	640447	23.51%	2.967%
14	10.016	1346	1348	1355	rVB	234426	204408	7.50%	0.947%
15	10.228	1380	1384	1391	rVB5	24003	38199	1.40%	0.177%
16	10.533	1433	1436	1442	rVB	118383	114422	4.20%	0.530%
17	10.616	1446	1450	1452	rBV3	48862	54746	2.01%	0.254%
18	10.780	1474	1478	1491	rBV	1498146	1393058	51.14%	6.455%
19	10.880	1491	1495	1503	rVB	73843	85470	3.14%	0.396%
20	11.480	1593	1597	1600	rBV	614583	525153	19.28%	2.433%
21	11.980	1679	1682	1687	rBV	90410	93916	3.45%	0.435%
22	13.063	1862	1866	1869	rBV	1818936	1559067	57.24%	7.224%
23	13.269	1894	1901	1904	rBV4	26937	42996	1.58%	0.199%
24	13.939	2011	2015	2021	rBV	231500	278559	10.23%	1.291%
25	14.127	2044	2047	2054	rBV	429355	441298	16.20%	2.045%
26	14.574	2118	2123	2130	rBV3	58636	129704	4.76%	0.601%
27	14.874	2172	2174	2178	rVB	29797	27454	1.01%	0.127%
28	15.227	2231	2234	2238	rVB	45316	46414	1.70%	0.215%
29	15.627	2299	2302	2303	rBV	30273	38636	1.42%	0.179%
30	15.657	2303	2307	2310	rVV	242020	331875	12.18%	1.538%
31	15.692	2310	2313	2319	rVB	88821	117480	4.31%	0.544%
32	16.080	2375	2379	2383	rVB2	41908	64185	2.36%	0.297%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110646.D
Acq On : 9 Nov 2018 23:52
Operator : JU/SJ
Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

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-BF110818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

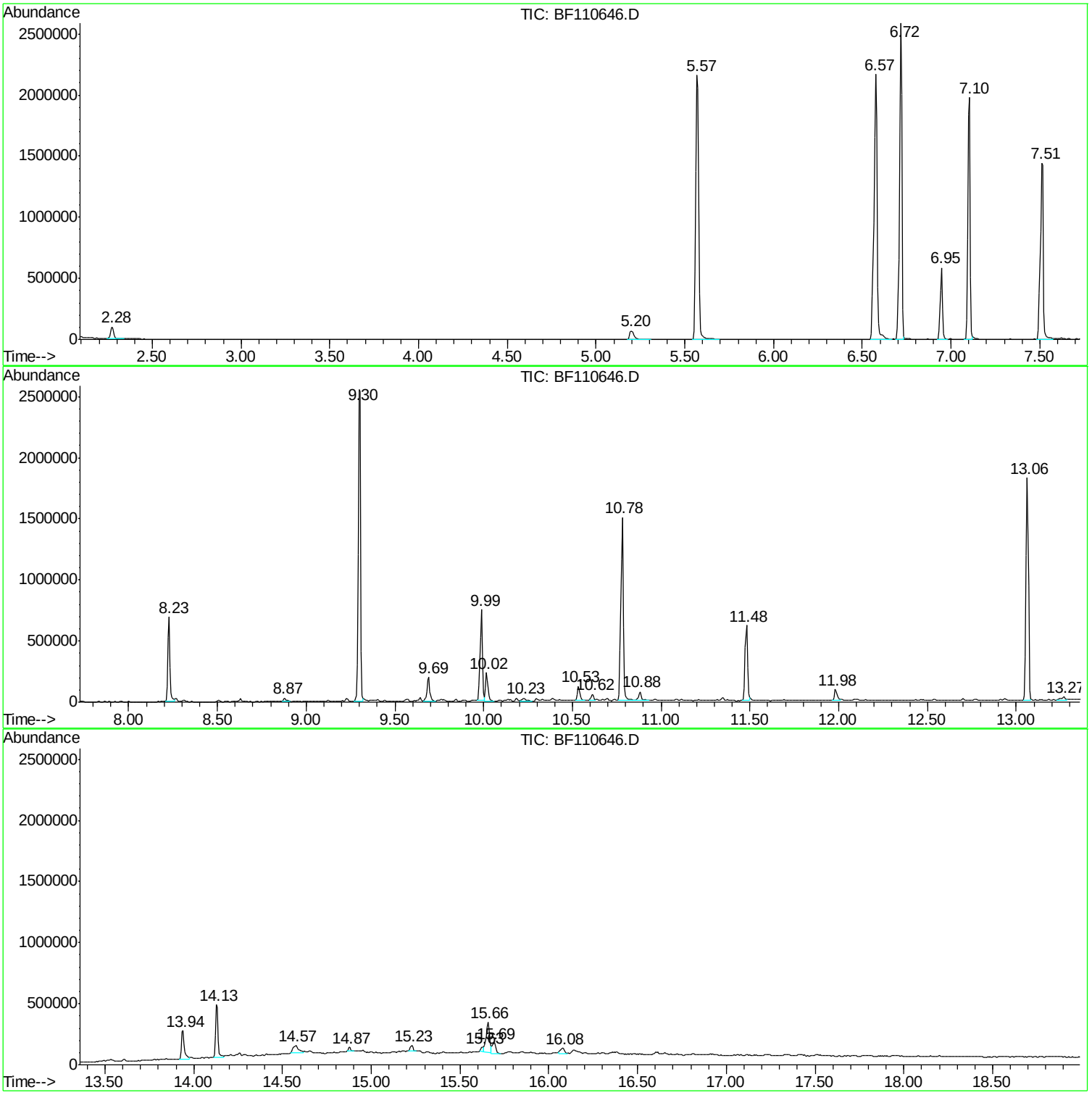
Sum of corrected areas: 21582438

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110646.D
Acq On : 9 Nov 2018 23:52
Operator : JU/SJ
Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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\BF110918\
Data File : BF110646.D
Acq On : 9 Nov 2018 23:52
Operator : JU/SJ
Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

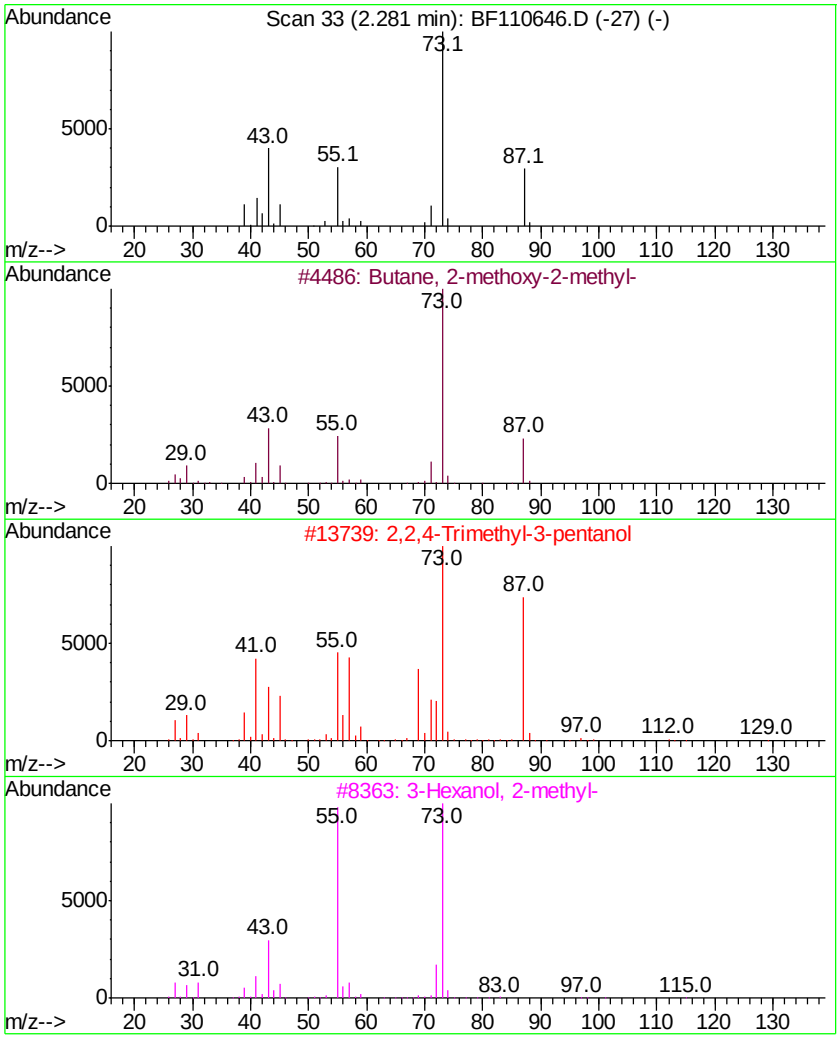
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

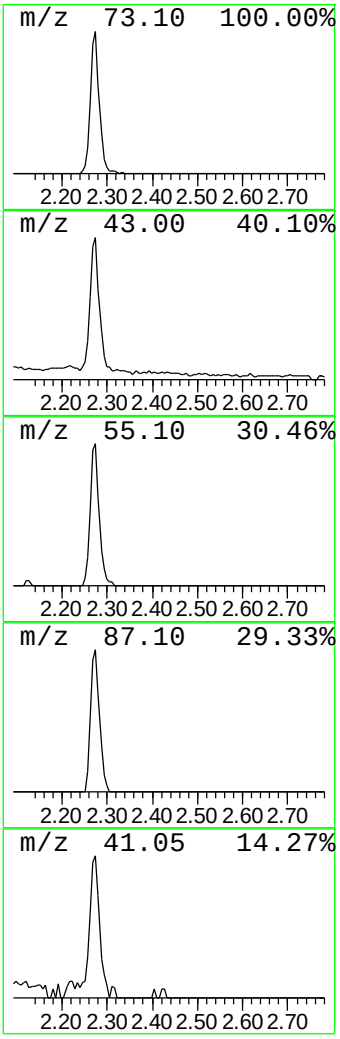
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.28	5.45 ng	131881	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110646.D
Acq On : 9 Nov 2018 23:52
Operator : JU/SJ
Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

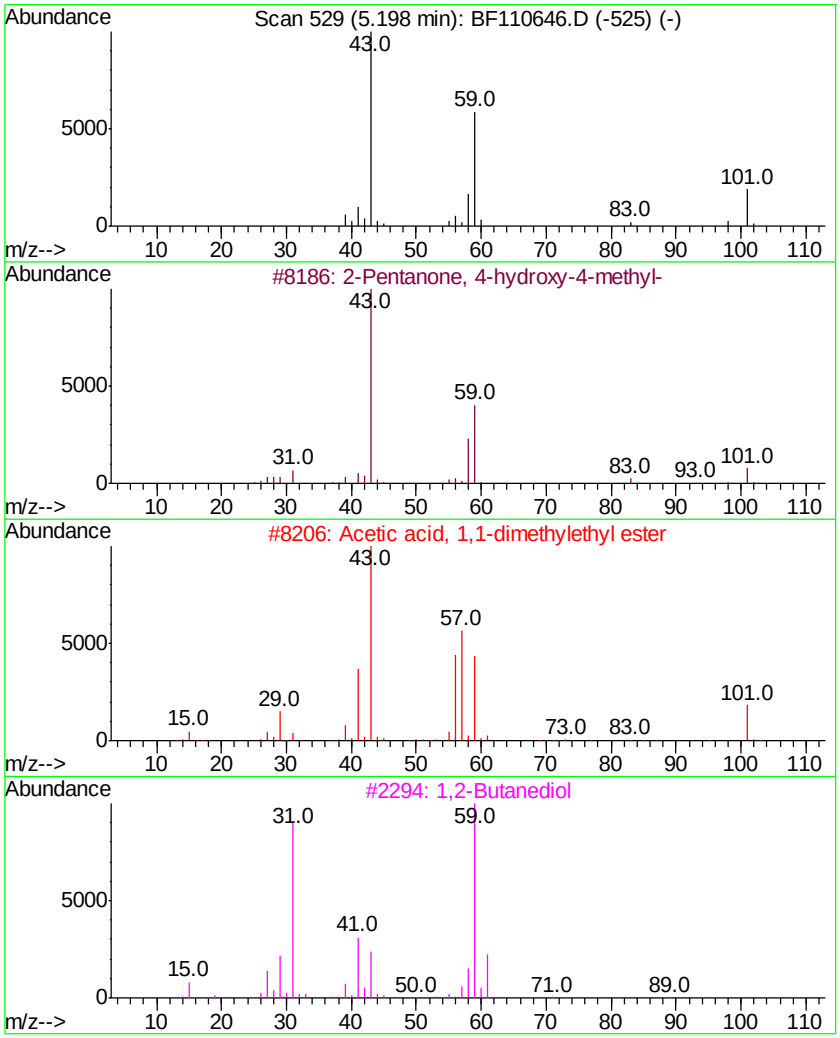
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

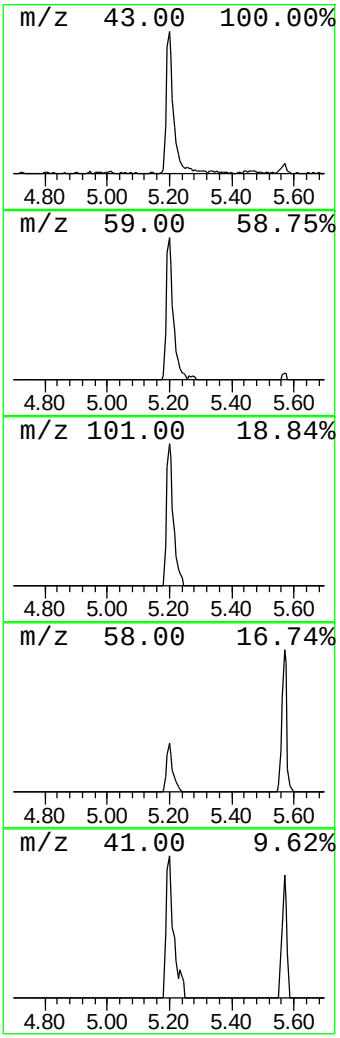
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	4.55 ng	110099	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	1,2-Butanediol	90	C4H10O2	000584-03-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110646.D
Acq On : 9 Nov 2018 23:52
Operator : JU/SJ
Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

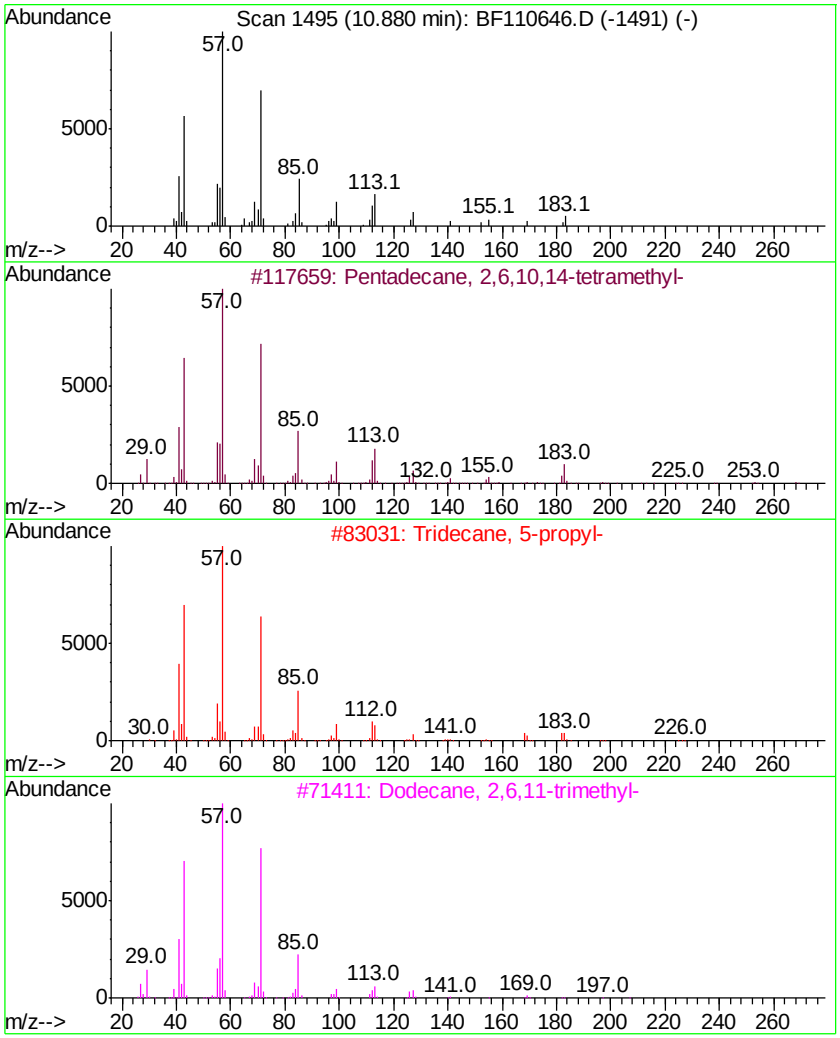
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

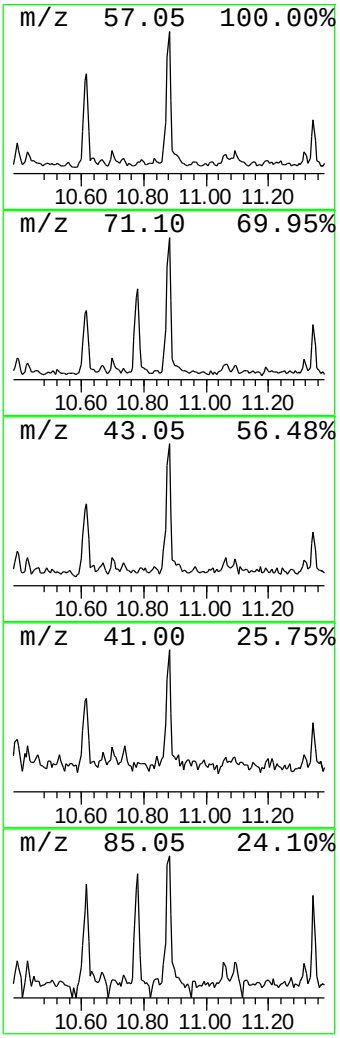
****

Peak Number 5 Pentadecane, 2,6,10,14-tetr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	3.26 ng	85470	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	91
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	80
3	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
5	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
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Operator : JU/SJ
Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

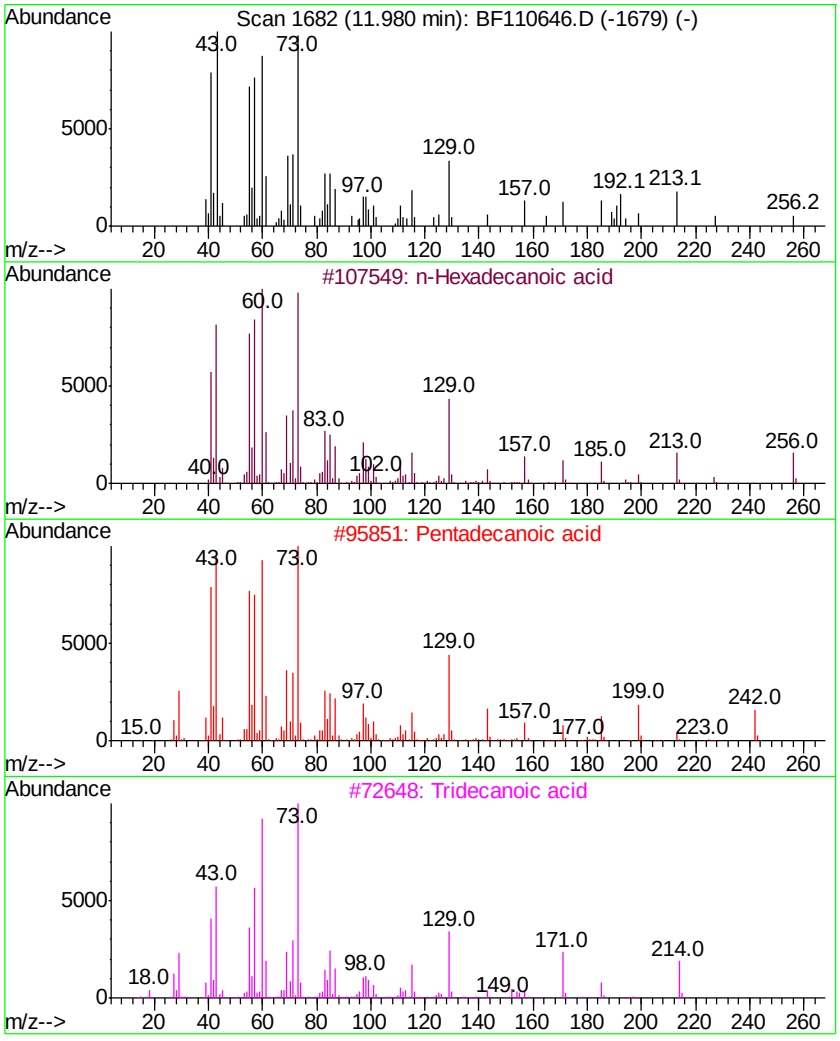
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

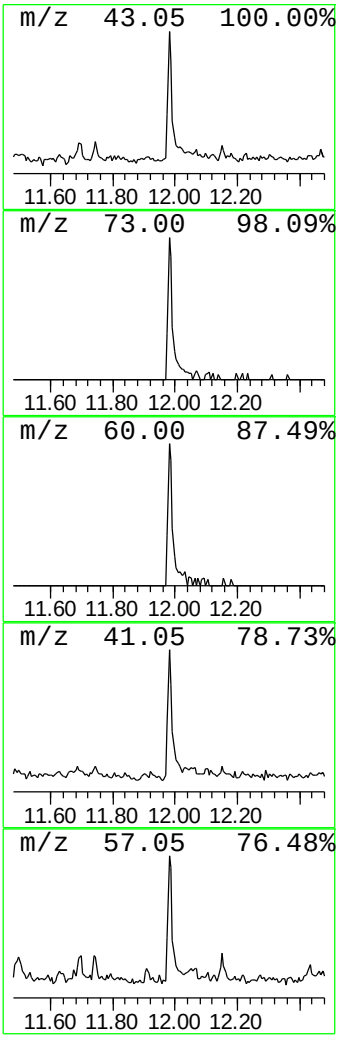
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	3.58 ng	93916	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





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Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

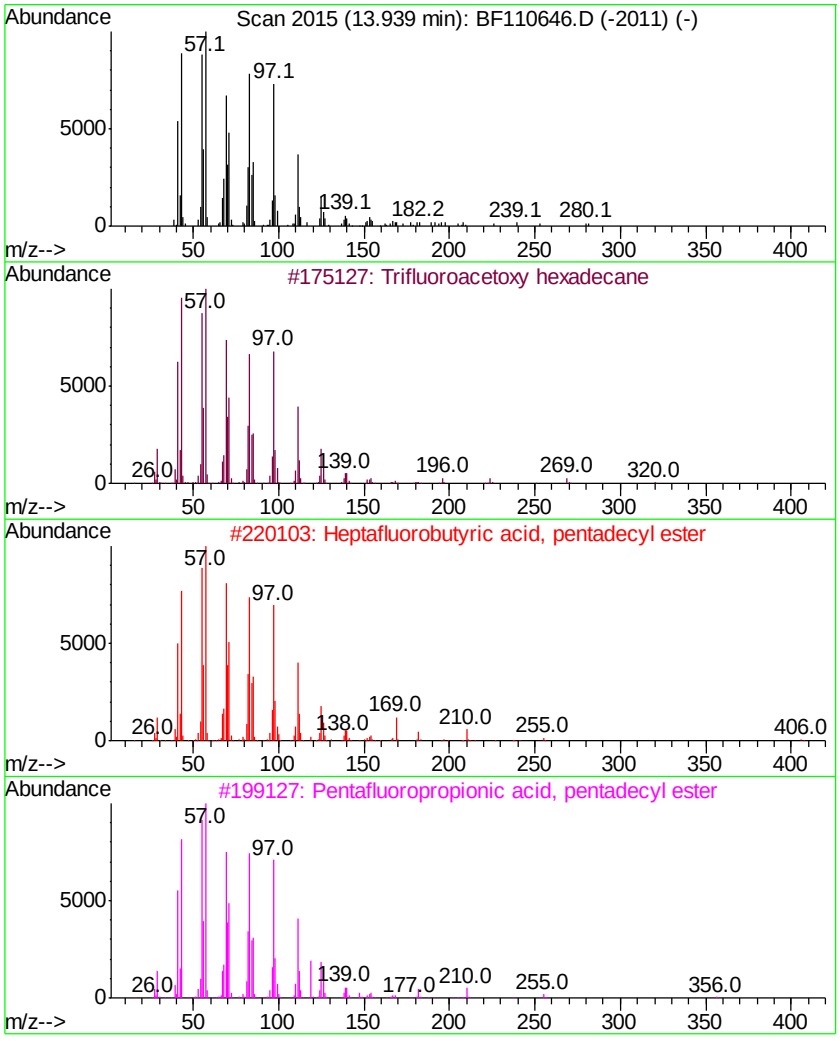
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

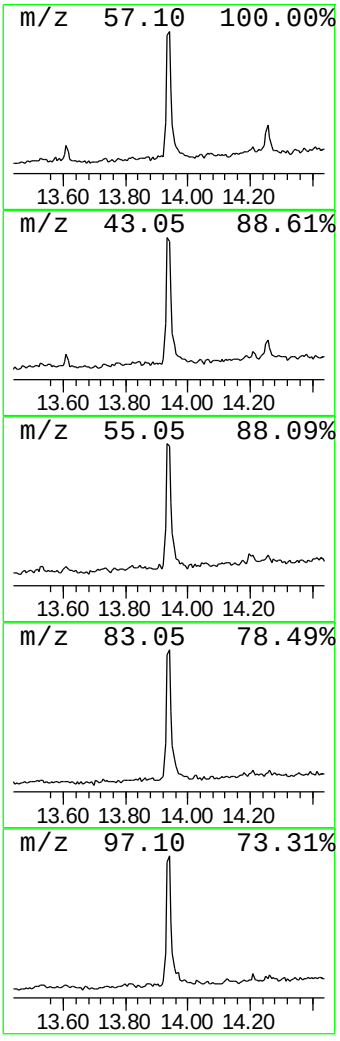
****

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	12.62 ng	278559	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93





Library Search Compound Report

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Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

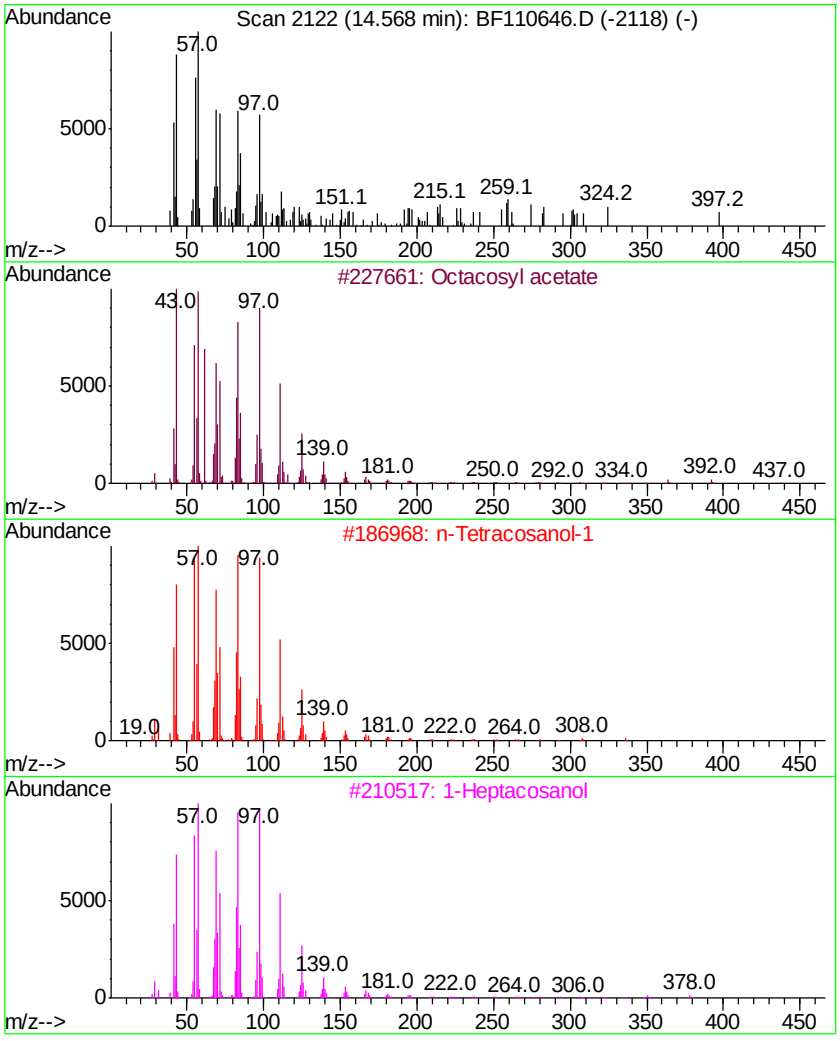
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

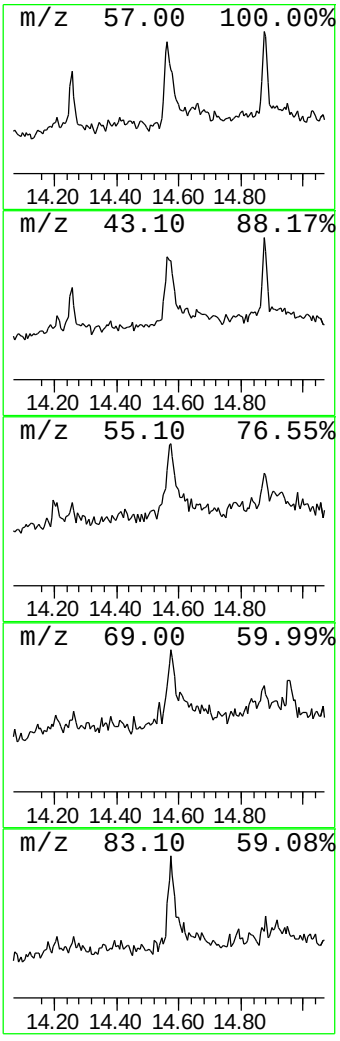
****

Peak Number 8 Octacosyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	5.88 ng	129704	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl acetate	452	C30H60O2	018206-97-8	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	90
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





Library Search Compound Report

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Acq On : 9 Nov 2018 23:52
Operator : JU/SJ
Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

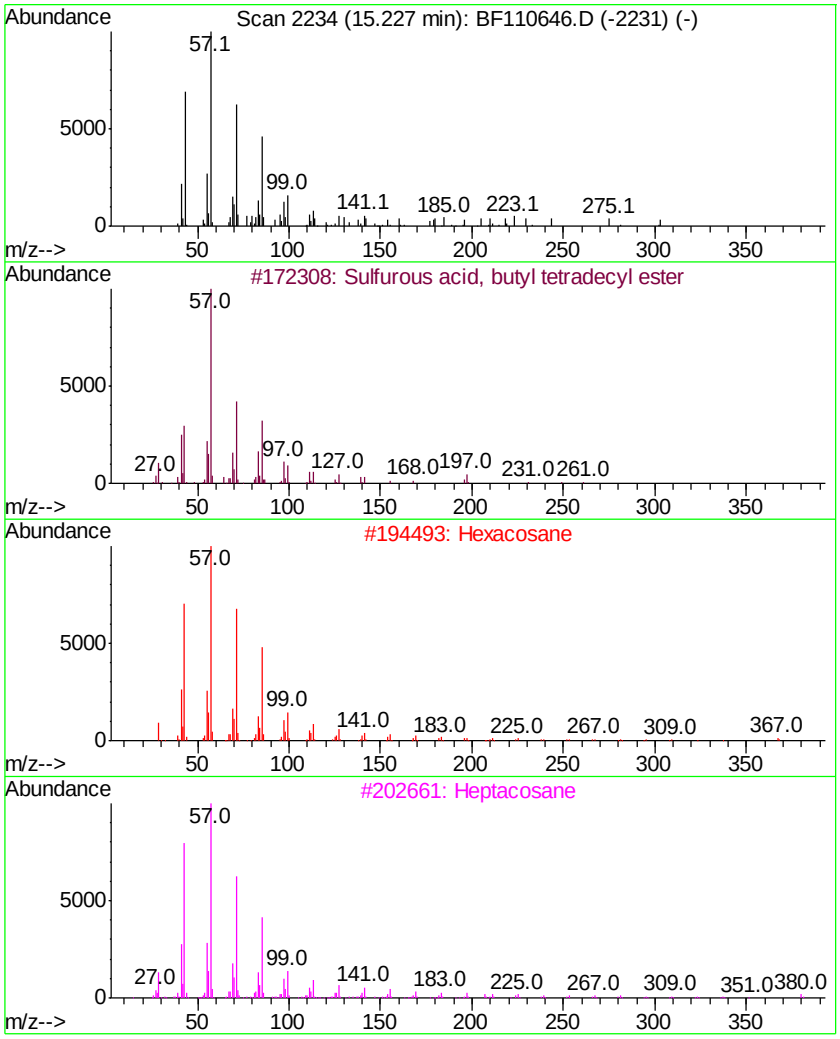
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

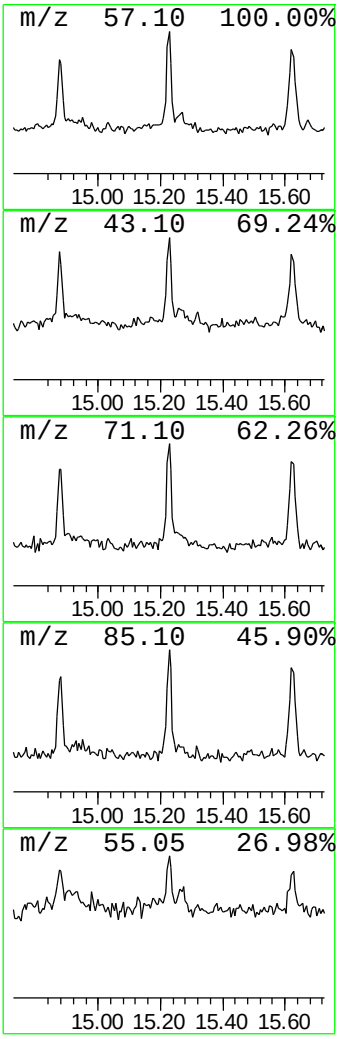
****

Peak Number 9 Sulfurous acid, butyl tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	2.80 ng	46414	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80
2	Hexacosane	366	C26H54	000630-01-3	74
3	Heptacosane	380	C27H56	000593-49-7	74
4	Octacosane	394	C28H58	000630-02-4	74
5	Tetracosane	338	C24H50	000646-31-1	74





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Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

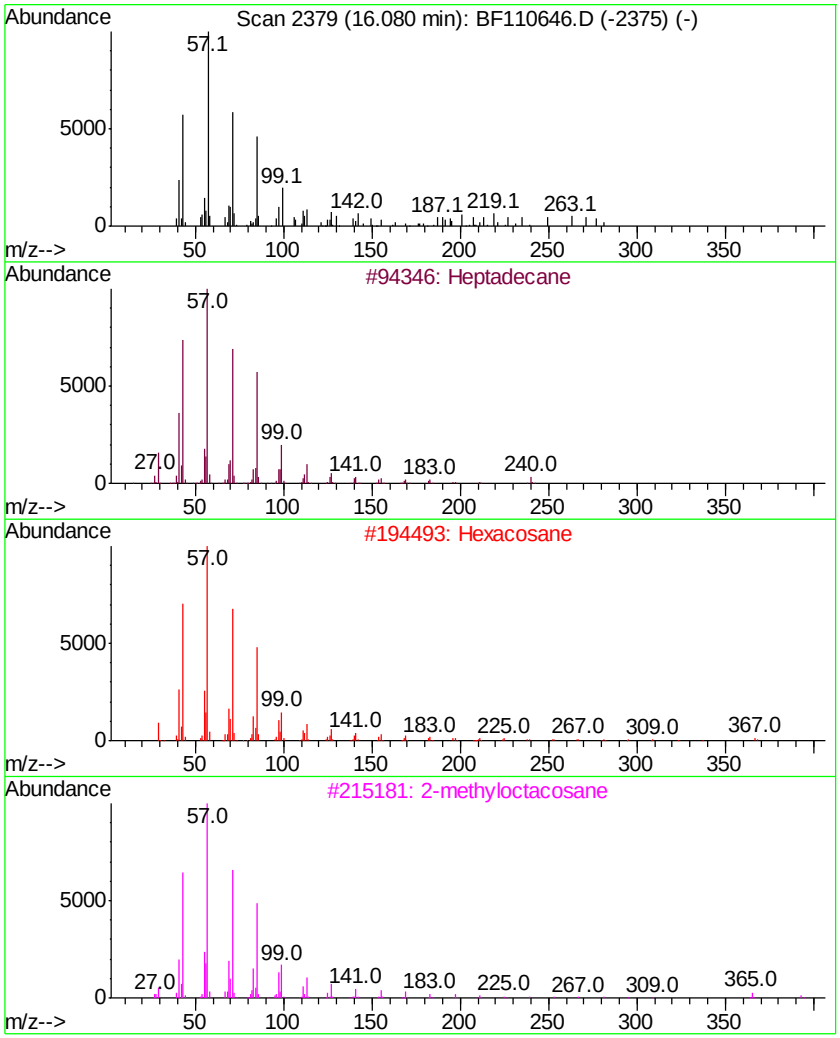
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

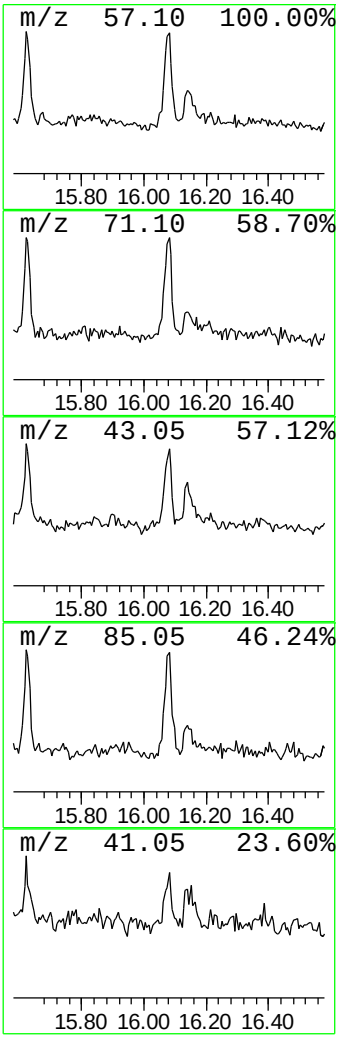
****

Peak Number 10 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	3.87 ng	64185	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	72
2	Hexacosane	366	C26H54	000630-01-3	59
3	2-methyloctacosane	408	C29H60	1000376-72-8	59
4	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	53
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110918\
Data File : BF110646.D
Acq On : 9 Nov 2018 23:52
Operator : JU/SJ
Sample : J5884-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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...	2.28	5.5	ng	131881	1	6.95	483572	20.0
2-Pentanone, 4-hy...	5.20	4.5	ng	110099	1	6.95	483572	20.0
Pentadecane, 2,6,...	10.88	3.3	ng	85470	4	11.48	525153	20.0
n-Hexadecanoic acid	11.98	3.6	ng	93916	4	11.48	525153	20.0
Trifluoroacetoxy ...	13.94	12.6	ng	278559	5	14.13	441298	20.0
Octacosyl acetate	14.57	5.9	ng	129704	5	14.13	441298	20.0
Sulfurous acid, b...	15.23	2.8	ng	46414	6	15.66	331875	20.0
Heptadecane	16.08	3.9	ng	64185	6	15.66	331875	20.0