LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003763.D
Acq On : 27 Oct 2020 19:55
Operator : CG/JU
Sample : L4511-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : OB-9

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_P\METHODS\8270-BP101920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003763.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.252	52	62	72	rBV	176858	403307	2.85%	0.701%
2	3.346	72	78	95	rVB	719272	1096356	7.76%	1.906%
3	6.011	521	531	549	rBV	1329396	2013966	14.26%	3.501%
4	7.657	802	811	822	rBV	791746	1300050	9.20%	2.260%
5	8.510	948	956	963	rBV	643065	1023969	7.25%	1.780%
6	9.681	1141	1155	1166	rBV	2152321	3645688	25.80%	6.338%
7	11.351	1429	1439	1447	rBV	815369	1381771	9.78%	2.402%
8	13.740	1836	1845	1852	rBV	6179791	8887334	62.91%	15.450%
9	13.992	1882	1888	1903	rVB	654756	958343	6.78%	1.666%
10	14.528	1973	1979	1989	rBV	546068	748824	5.30%	1.302%
11	15.110	2068	2078	2085	rBV	1336214	1965920	13.91%	3.418%
12	16.192	2256	2262	2277	rBV	553104	712904	5.05%	1.239%
13	16.586	2321	2329	2344	rBV	4787368	6813794	48.23%	11.845%
14	17.828	2534	2540	2547	rBV	1652757	2381901	16.86%	4.141%
15	18.092	2580	2585	2592	rBV	172931	213696	1.51%	0.371%
16	18.645	2673	2679	2686	rBV	619850	847903	6.00%	1.474%
17	19.445	2811	2815	2823	rBV	368368	460572	3.26%	0.801%
18	19.751	2863	2867	2871	rVB	219450	233312	1.65%	0.406%
19	19.839	2878	2882	2893	rBV	149263	217841	1.54%	0.379%
20	20.304	2955	2961	2966	rBV	11717013	14128100	100.00%	24.561%
21	20.527	2995	2999	3002	rBV	233603	281444	1.99%	0.489%
22	21.033	3080	3085	3089	rBV2	110616	148035	1.05%	0.257%
23	21.474	3155	3160	3170	rBV	1728906	2087731	14.78%	3.629%
24	21.845	3218	3223	3232	rVB	1940924	2635032	18.65%	4.581%
25	21.933	3235	3238	3248	rVB2	99100	142422	1.01%	0.248%
26	24.421	3654	3661	3672	rVB	1173076	2439603	17.27%	4.241%
27	25.033	3759	3765	3775	rVB	157034	352974	2.50%	0.614%

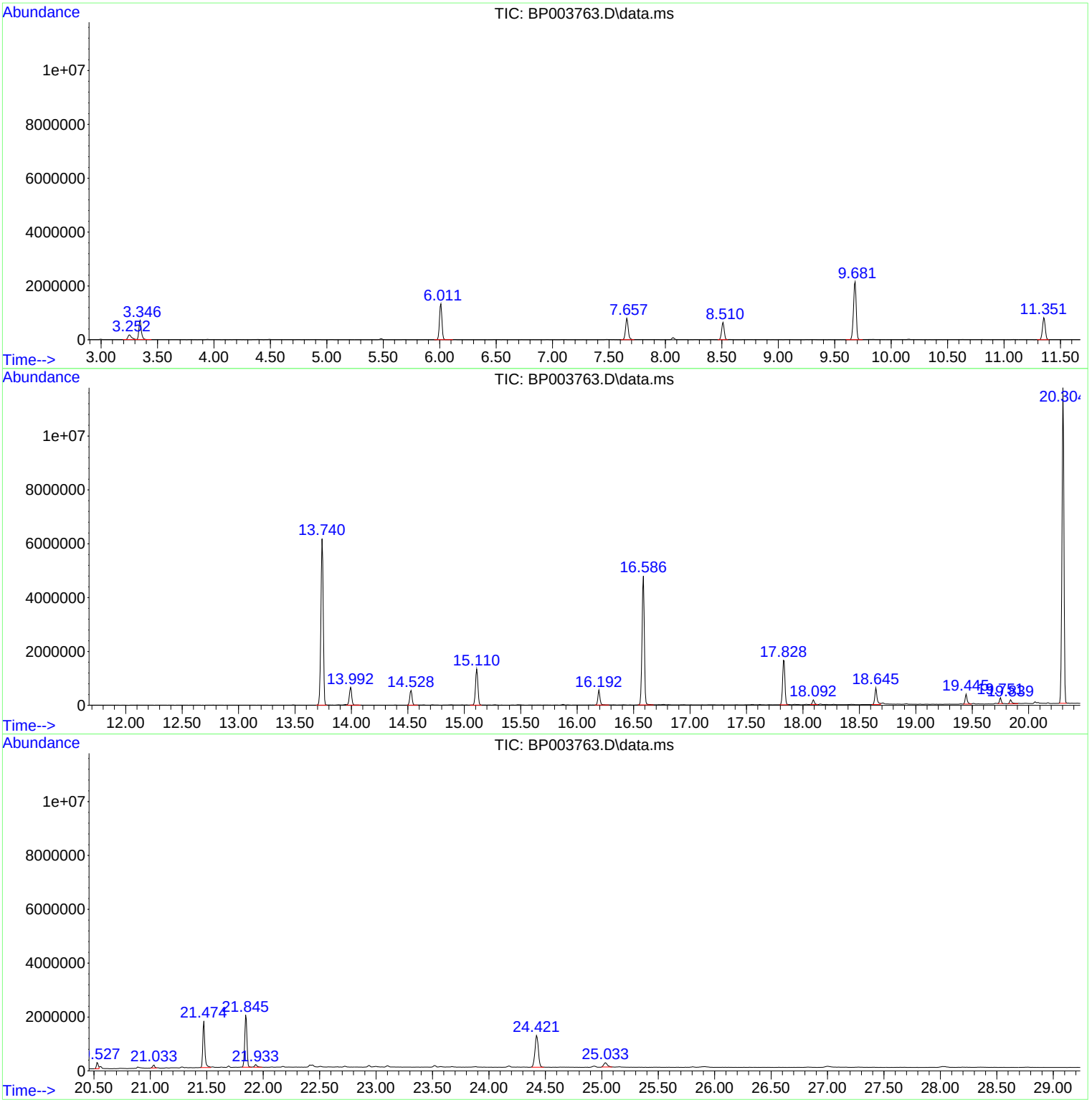
Sum of corrected areas: 57522792

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003763.D
Acq On : 27 Oct 2020 19:55
Operator : CG/JU
Sample : L4511-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OB-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.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_P\Data\BP102720\
Data File : BP003763.D
Acq On : 27 Oct 2020 19:55
Operator : CG/JU
Sample : L4511-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OB-9

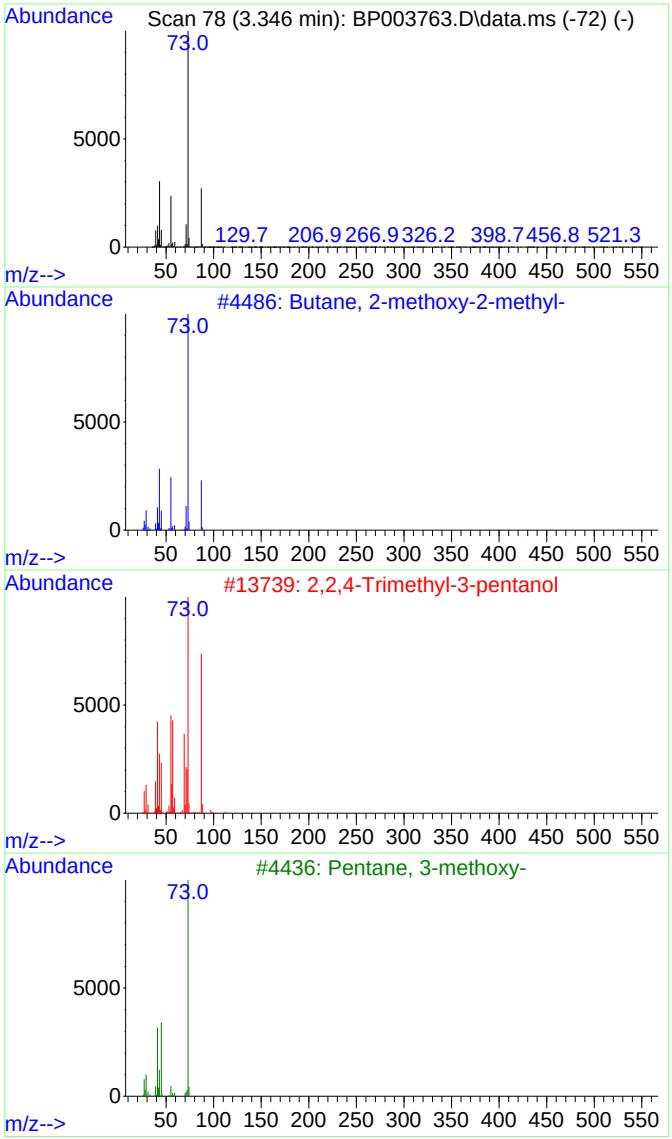
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

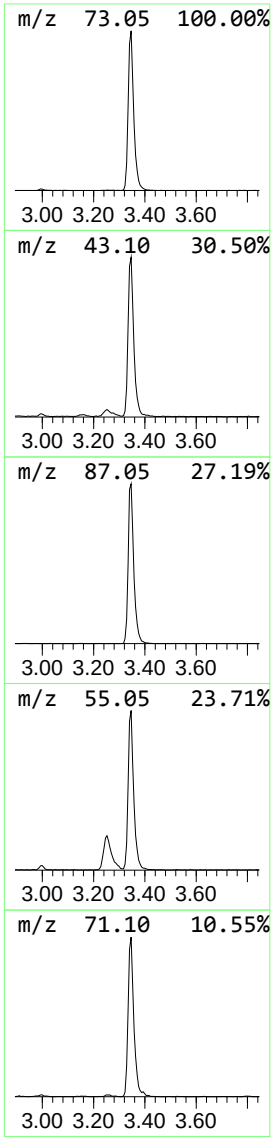
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.346	21.41 ng	1096360	1,4-Dichlorobenzene-d4	8.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003763.D
Acq On : 27 Oct 2020 19:55
Operator : CG/JU
Sample : L4511-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OB-9

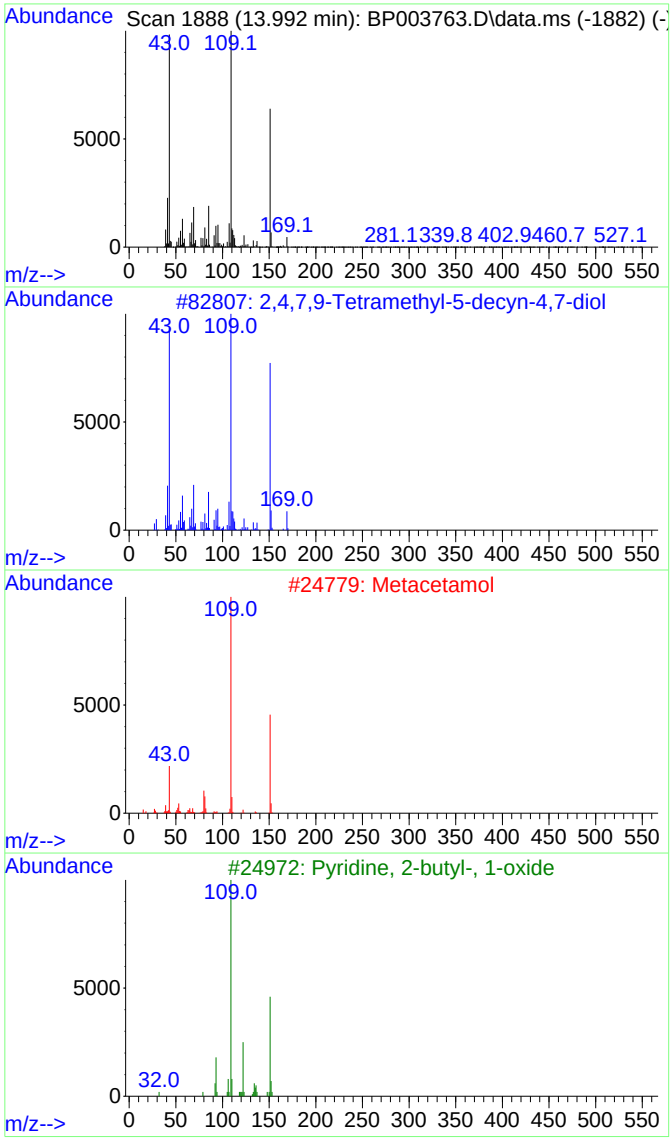
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

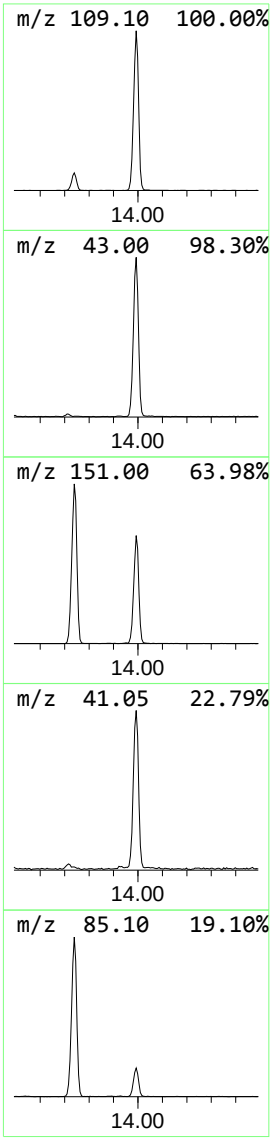
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	9.75 ng	958343	Acenaphthene-d10	15.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	52
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	50
4	Acetaminophen	151	C8H9NO2	000103-90-2	50
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003763.D
Acq On : 27 Oct 2020 19:55
Operator : CG/JU
Sample : L4511-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : OB-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

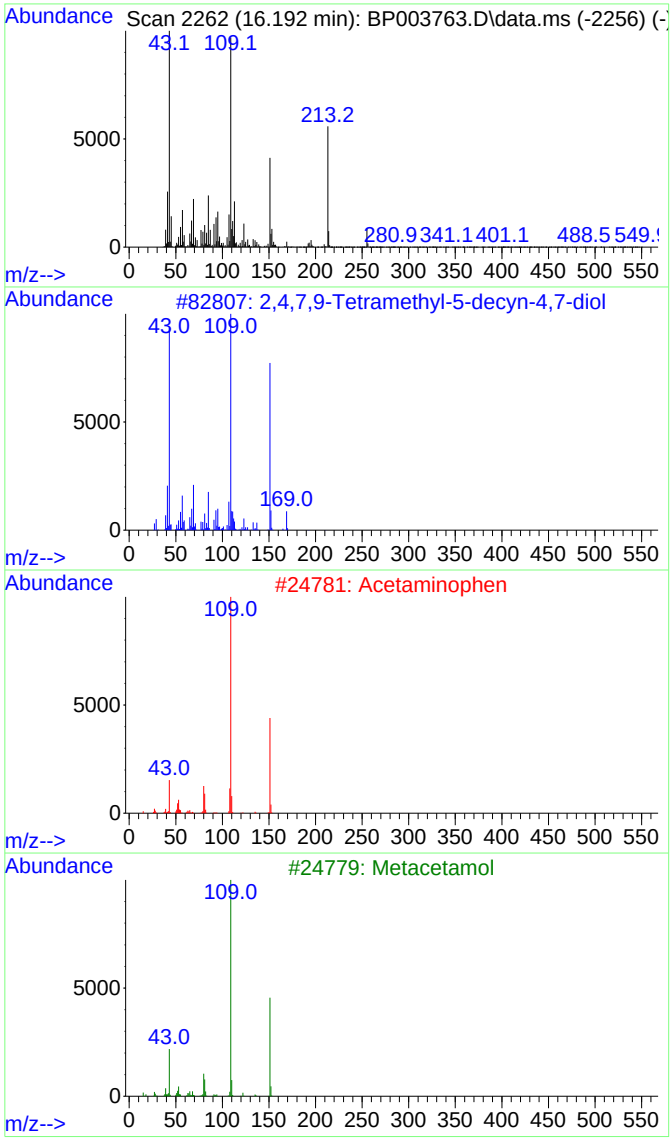
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

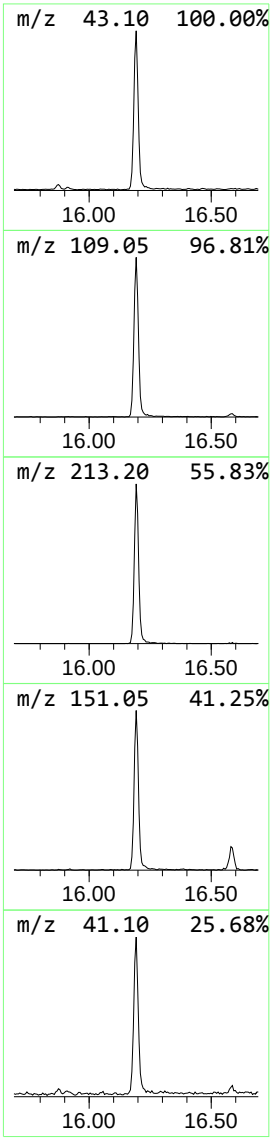
****

Peak Number 4 unknown16.192 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.192	7.25 ng	712904	Acenaphthene-d10	15.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	53
2	Acetaminophen	151	C8H9NO2	000103-90-2	38
3	Metacetamol	151	C8H9NO2	000621-42-1	38
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	38
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003763.D
Acq On : 27 Oct 2020 19:55
Operator : CG/JU
Sample : L4511-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : OB-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

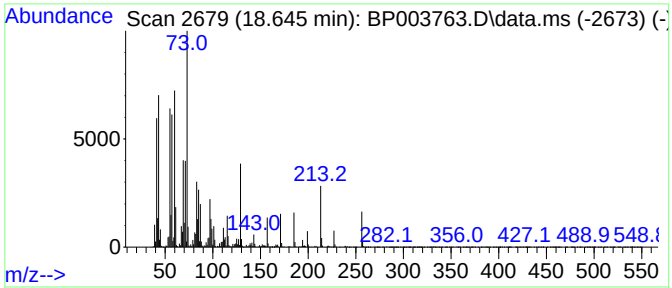
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

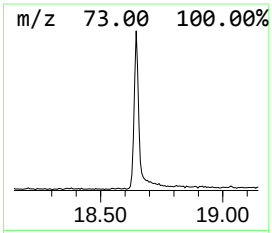
****

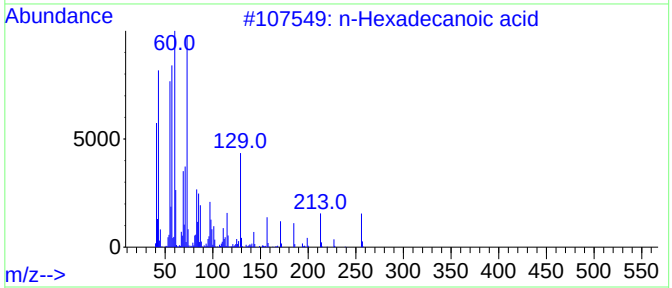
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

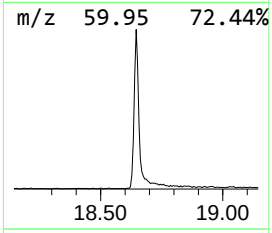
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.645	7.12 ng	847903	Phenanthrene-d10	17.828

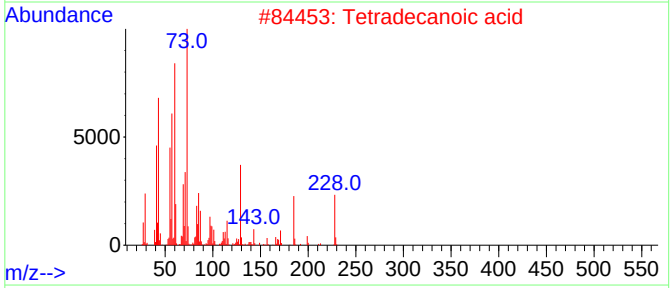
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
5	Octadecanoic acid	284	C18H36O2	000057-11-4	81

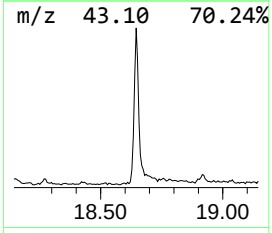


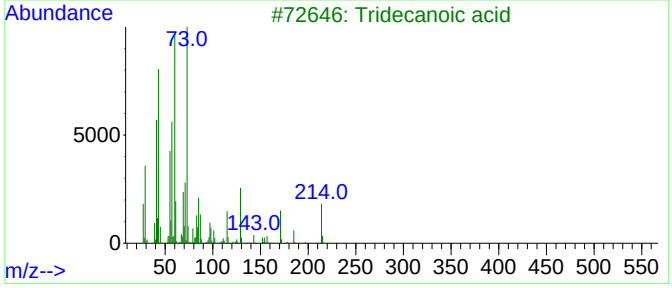


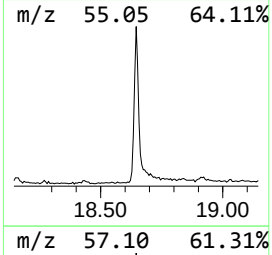


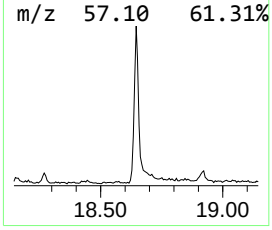












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003763.D
Acq On : 27 Oct 2020 19:55
Operator : CG/JU
Sample : L4511-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : OB-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

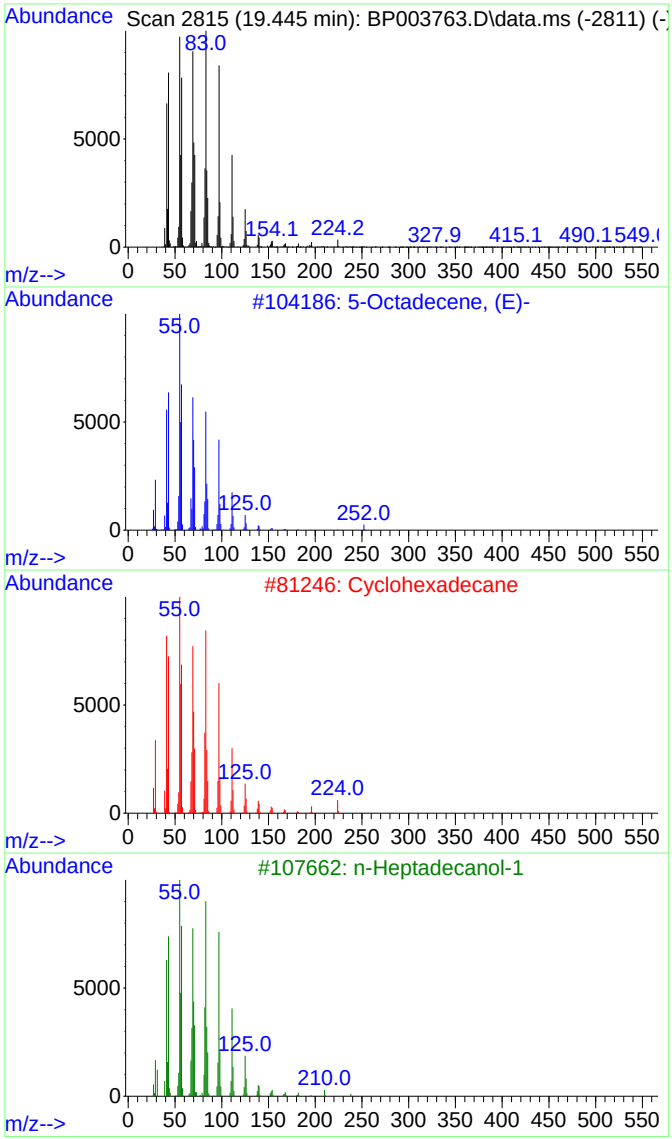
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

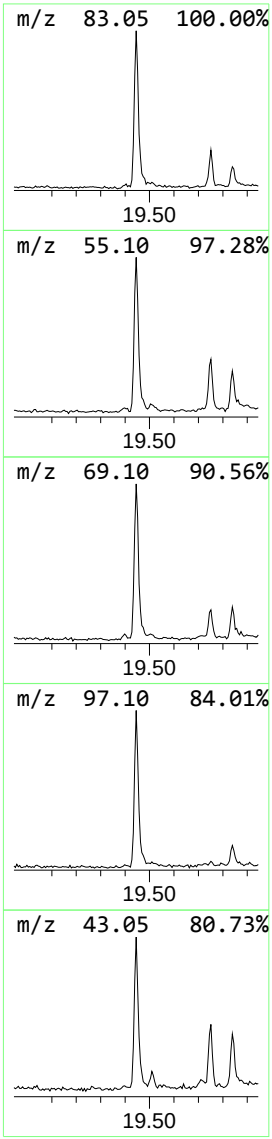
****

Peak Number 6 5-Octadecene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	3.87 ng	460572	Phenanthrene-d10	17.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	99
2	Cyclohexadecane	224	C16H32	000295-65-8	98
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Pentafluoropropionic acid, 4-hex...	388	C19H33F5O2	1000283-04-1	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003763.D
Acq On : 27 Oct 2020 19:55
Operator : CG/JU
Sample : L4511-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : OB-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

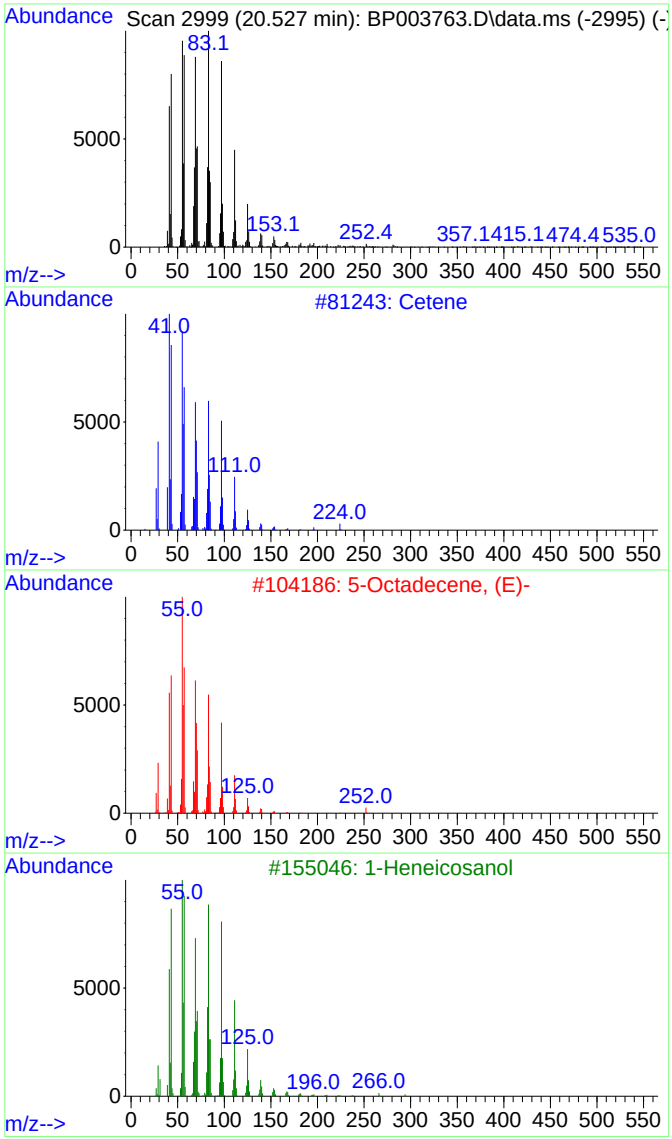
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

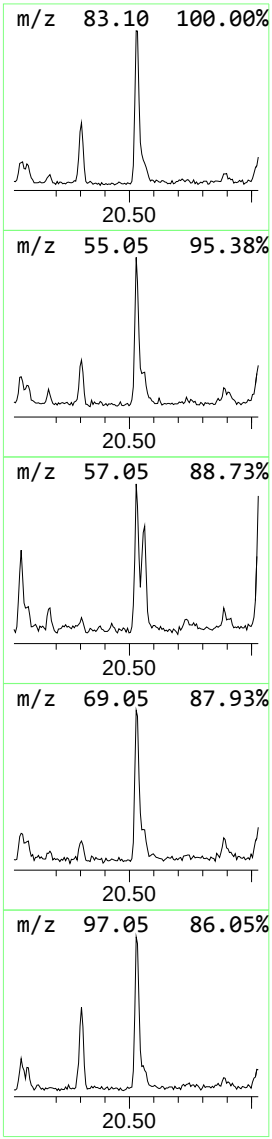
****

Peak Number 7 Cetene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.527	2.14 ng	281444	Chrysene-d12	21.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	96
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003763.D
Acq On : 27 Oct 2020 19:55
Operator : CG/JU
Sample : L4511-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : OB-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

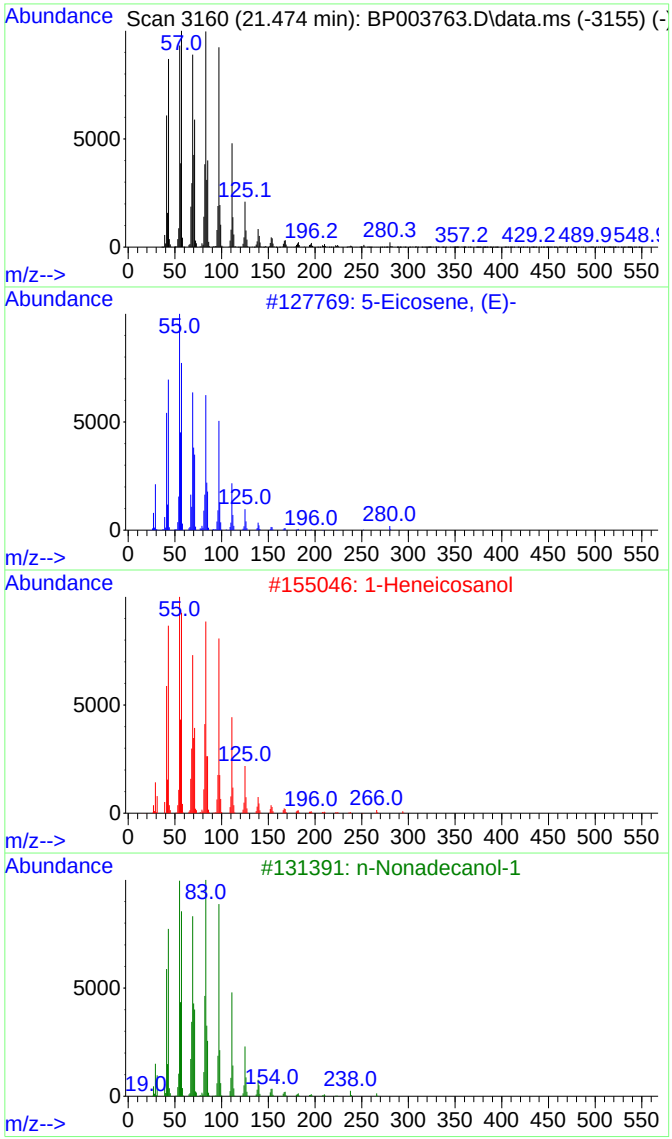
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

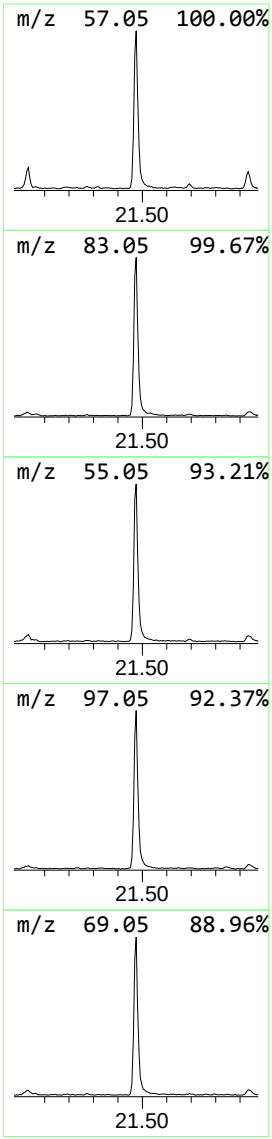
****

Peak Number 8 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.474	15.85 ng	2087730	Chrysene-d12	21.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003763.D
Acq On : 27 Oct 2020 19:55
Operator : CG/JU
Sample : L4511-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : OB-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

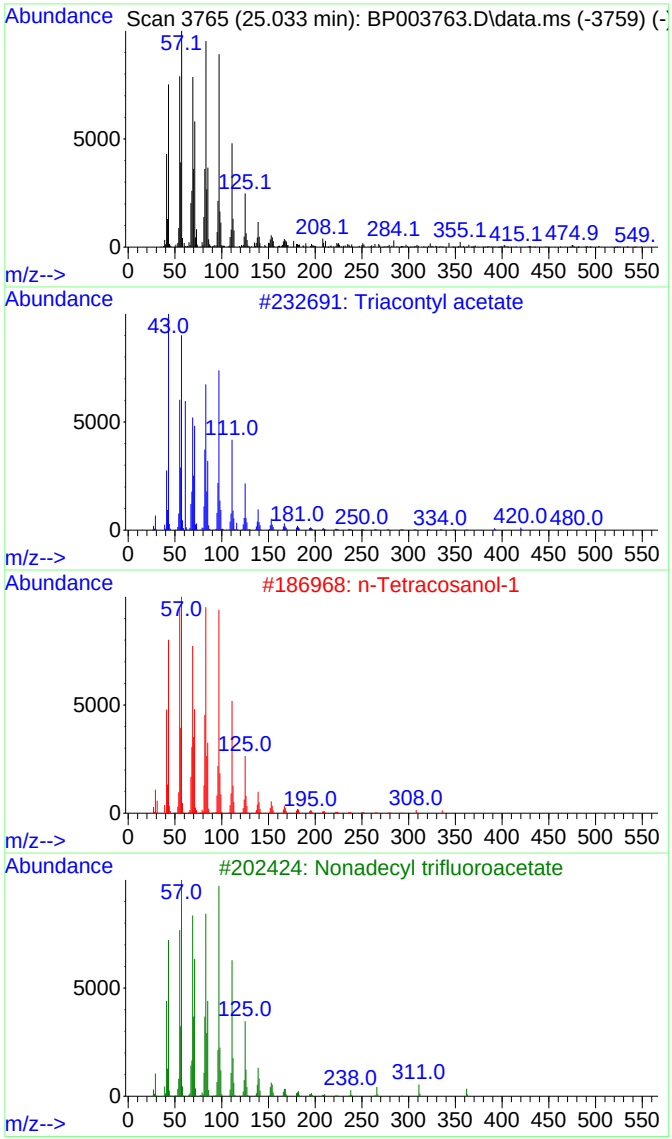
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

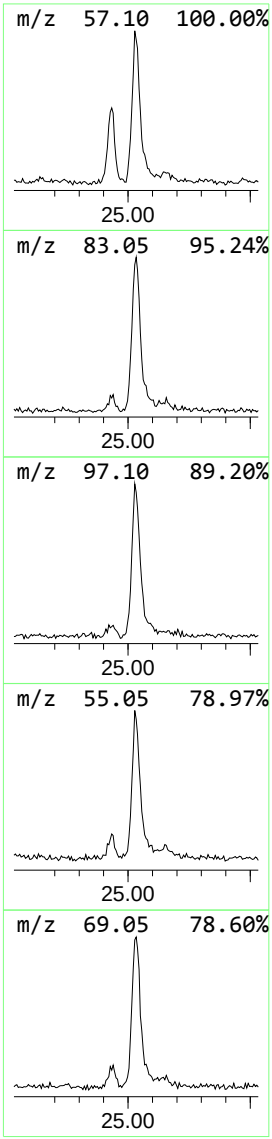
****

Peak Number 9 Triacontyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.033	2.89 ng	352974	Perylene-d12	24.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontyl acetate	480	C32H64O2	041755-58-2	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003763.D
Acq On : 27 Oct 2020 19:55
Operator : CG/JU
Sample : L4511-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : OB-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.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-metho...	3.346	21.4	ng	1096360	1	8.510	1023970	20.0
2,4,7,9-Tetrame...	13.992	9.8	ng	958343	3	15.110	1965920	20.0
unknown16.192	16.192	7.3	ng	712904	3	15.110	1965920	20.0
n-Hexadecanoic ...	18.645	7.1	ng	847903	4	17.828	2381900	20.0
5-Octadecene, (E)-	19.445	3.9	ng	460572	4	17.828	2381900	20.0
Cetene	20.527	2.1	ng	281444	5	21.845	2635030	20.0
5-Eicosene, (E)-	21.474	15.9	ng	2087730	5	21.845	2635030	20.0
Triacontyl acetate	25.033	2.9	ng	352974	6	24.421	2439600	20.0