LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122371.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	5	11	22	rVB	938461	1254876	13.66%	2.104%
2	2.234	22	25	39	rVB2	54401	111053	1.21%	0.186%
3	4.457	398	403	409	rBV	898952	1004444	10.93%	1.684%
4	5.081	502	509	520	rBV	299466	416480	4.53%	0.698%
5	5.481	571	577	580	rBV	6163656	6316819	68.75%	10.589%
6	6.487	742	748	751	rBV	5728275	6579873	71.61%	11.030%
7	6.687	779	782	797	rVB	151155	145682	1.59%	0.244%
8	6.863	809	812	816	rVB	1824550	1387840	15.10%	2.326%
9	7.428	902	908	911	rBV	4337771	4263457	46.40%	7.147%
10	8.145	1026	1030	1034	rBV	1931692	1830917	19.93%	3.069%
11	9.228	1209	1214	1217	rBV	8188973	7660094	83.37%	12.840%
12	9.616	1276	1280	1289	rBV	1412888	1161685	12.64%	1.947%
13	9.904	1324	1329	1339	rVB	2576542	2219609	24.16%	3.721%
14	10.692	1458	1463	1466	rBV	5788349	5353737	58.27%	8.974%
15	11.386	1577	1581	1585	rBV	2632135	2373799	25.84%	3.979%
16	11.921	1664	1672	1685	rBV	802879	972578	10.59%	1.630%
17	12.369	1745	1748	1752	rVB	286040	260878	2.84%	0.437%
18	12.704	1801	1805	1815	rBV	288095	388971	4.23%	0.652%
19	12.980	1846	1852	1855	rBV	9323240	9188199	100.00%	15.402%
20	13.874	2000	2004	2022	rBV	939199	1474174	16.04%	2.471%
21	14.027	2025	2030	2033	rBV	2916190	2532869	27.57%	4.246%
22	15.498	2274	2280	2284	rBV	1904584	2366670	25.76%	3.967%
23	15.539	2284	2287	2293	rVB	68519	94110	1.02%	0.158%
24	16.039	2366	2372	2380	rBV3	106671	297431	3.24%	0.499%

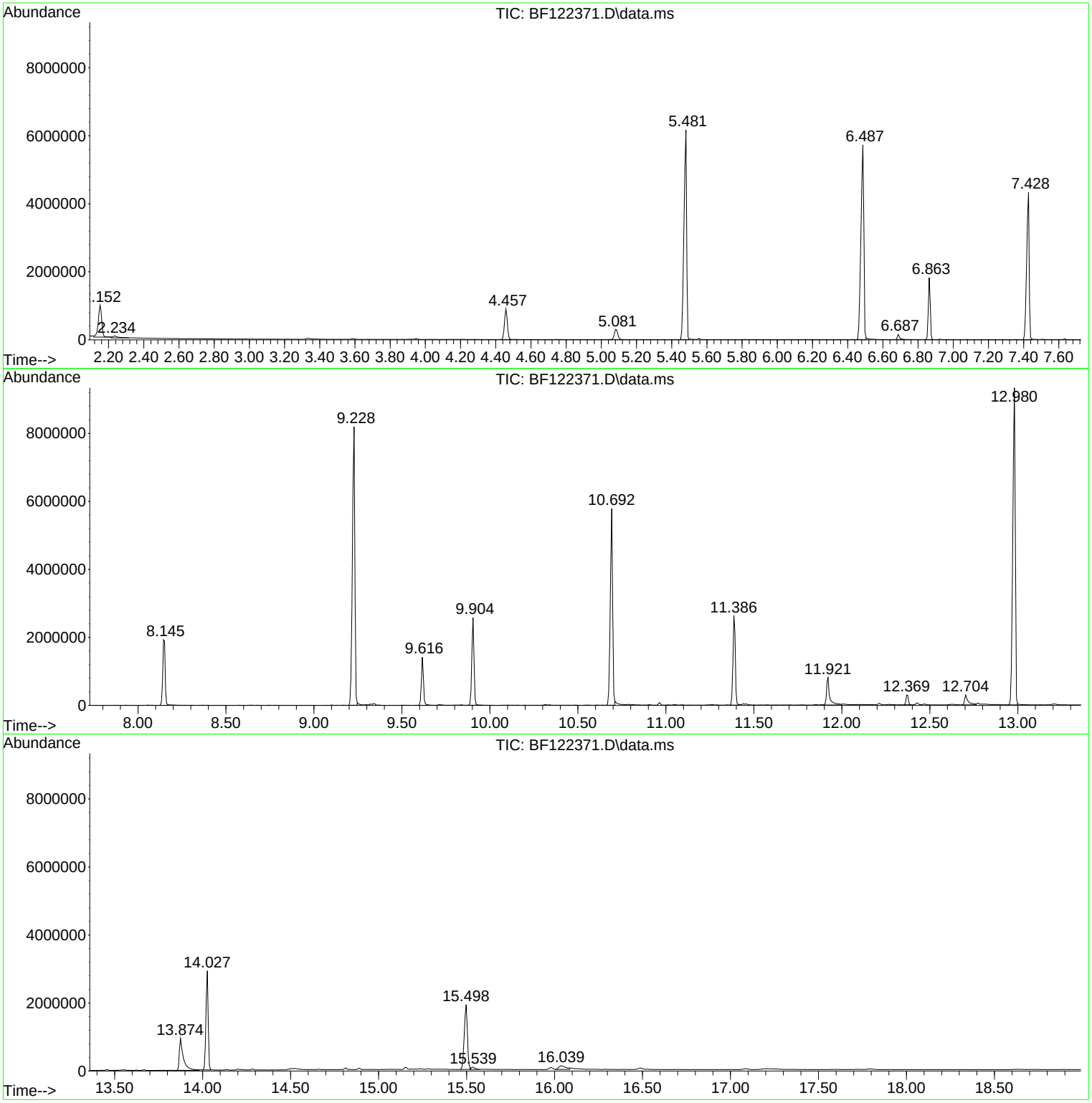
Sum of corrected areas: 59656245

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

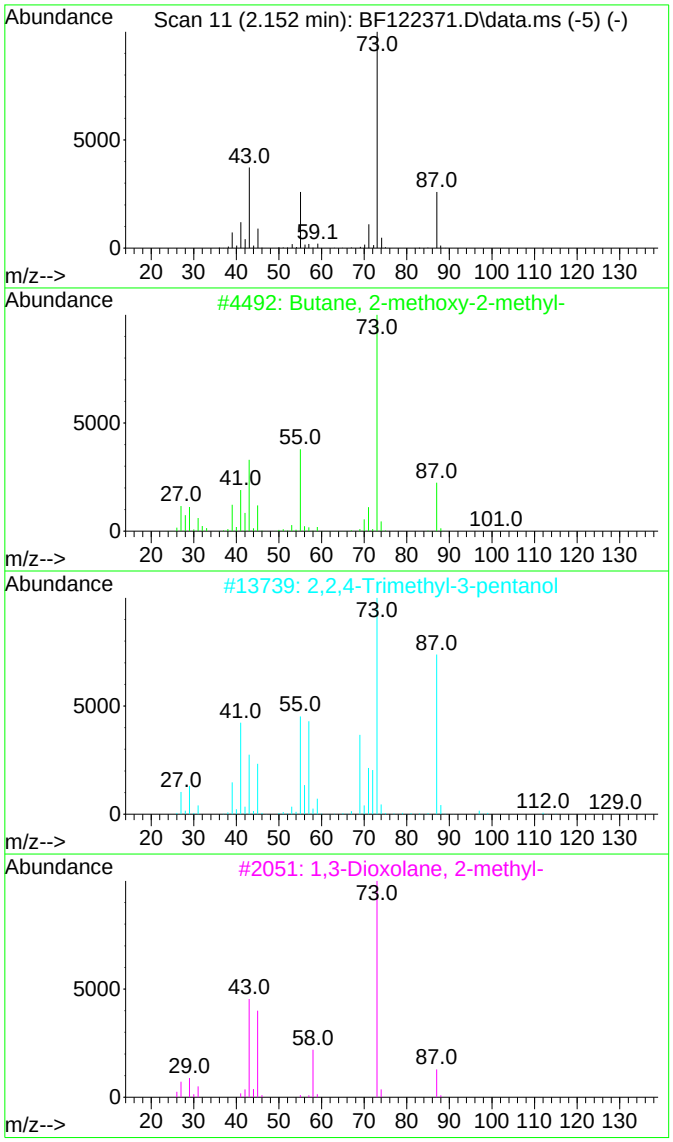
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

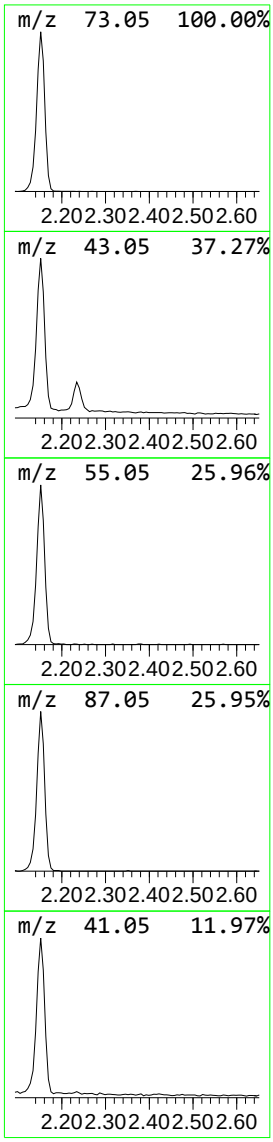
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	18.08 ng	1254880	1,4-Dichlorobenzene-d4	6.863

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

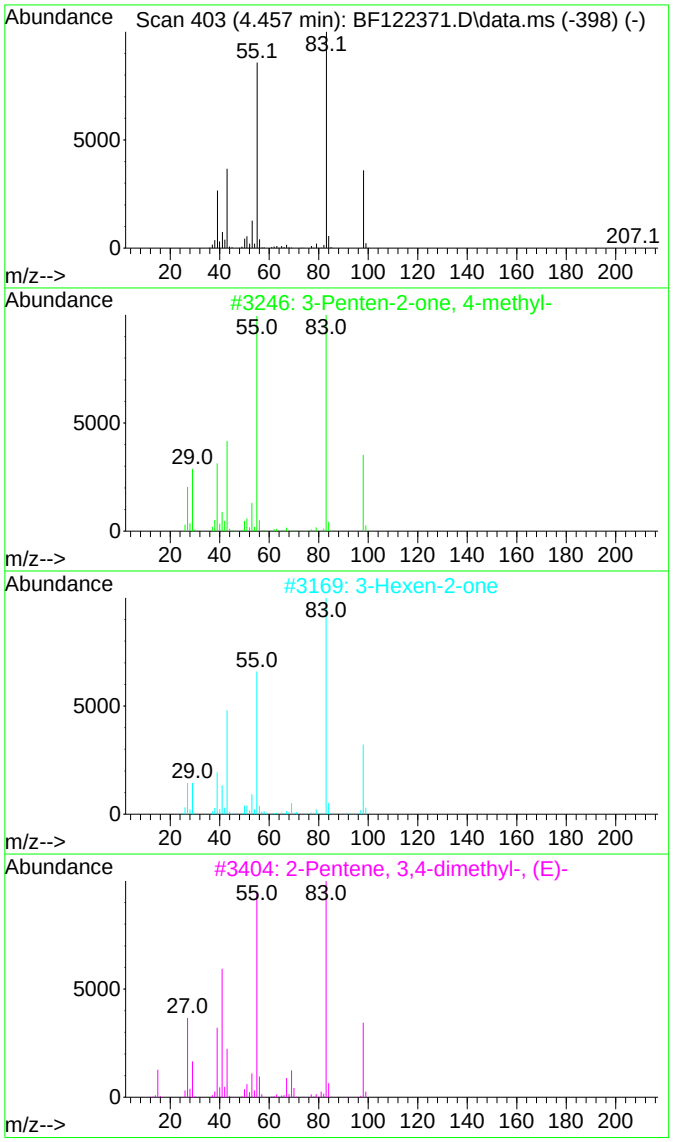
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

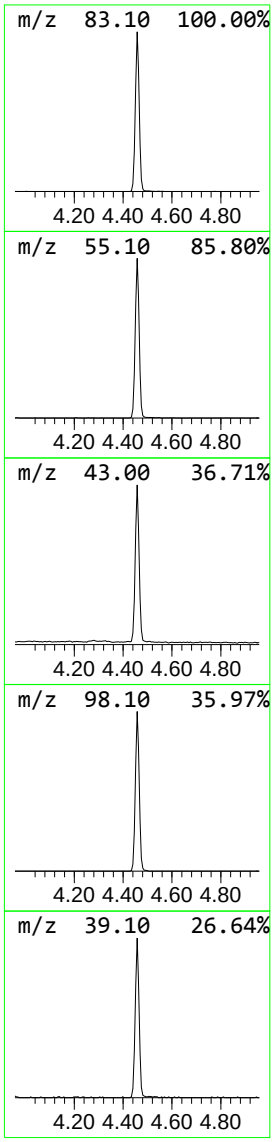
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	14.47 ng	1004440	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

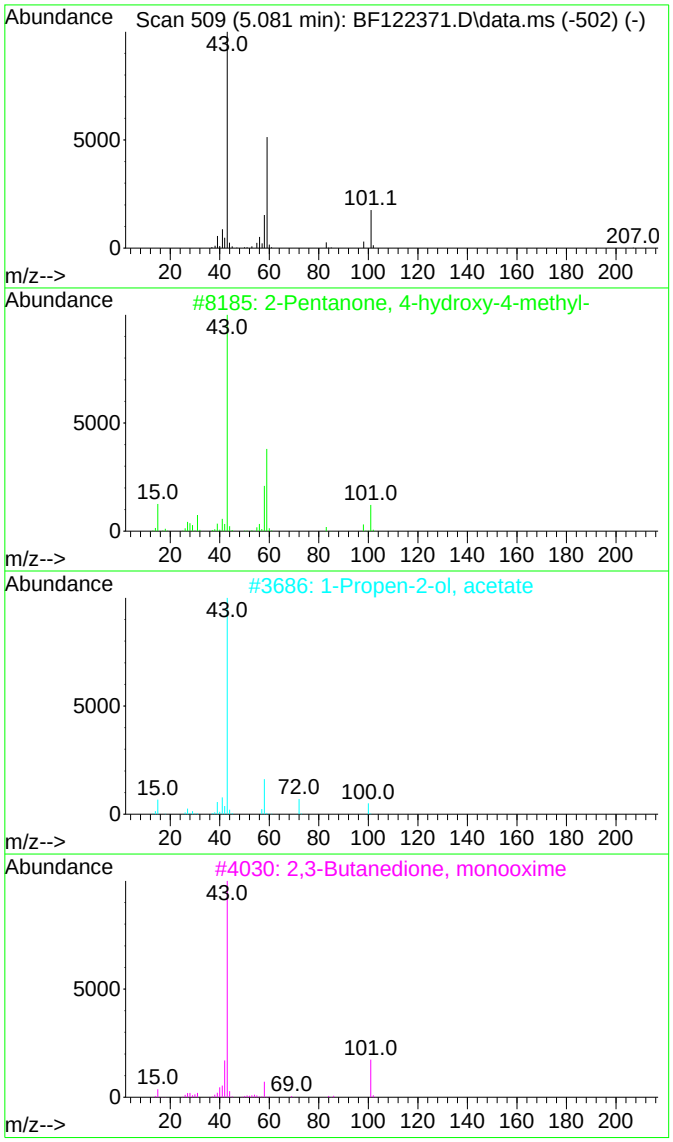
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

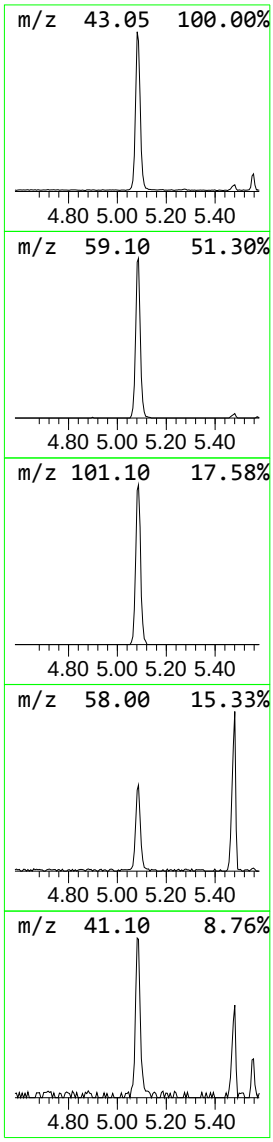
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	6.00 ng	416480	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

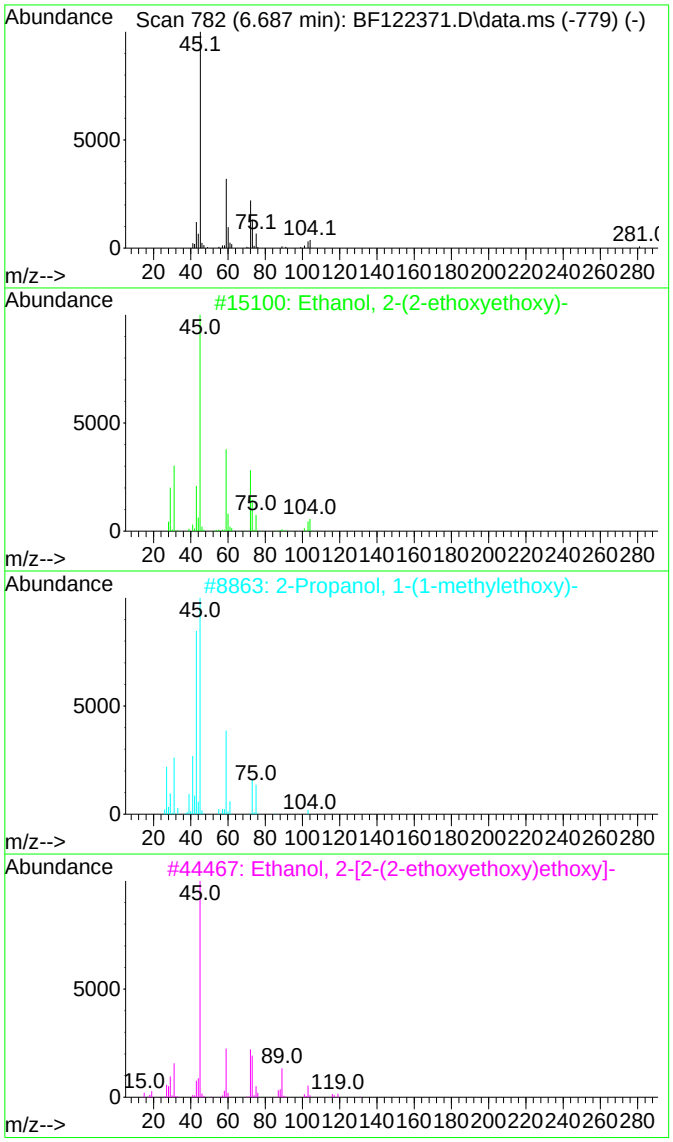
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

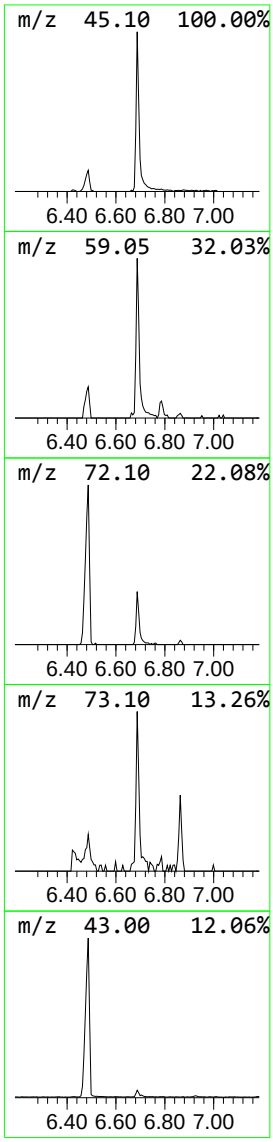
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.687	2.10 ng	145682	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	39
4	Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	37
5	.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

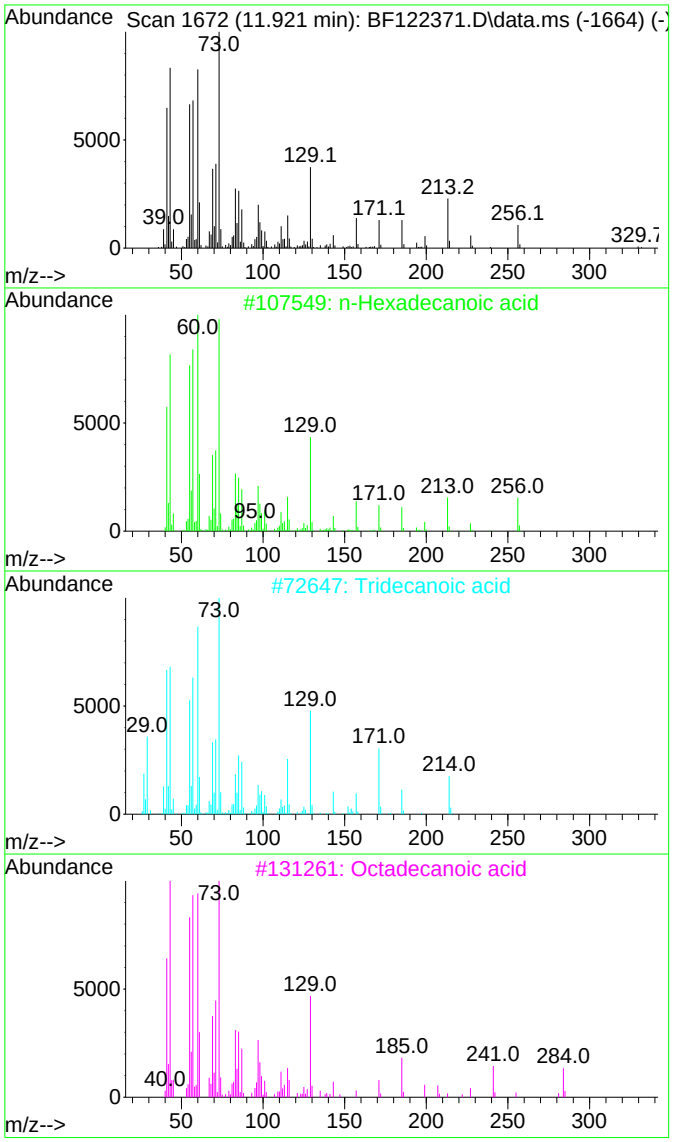
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

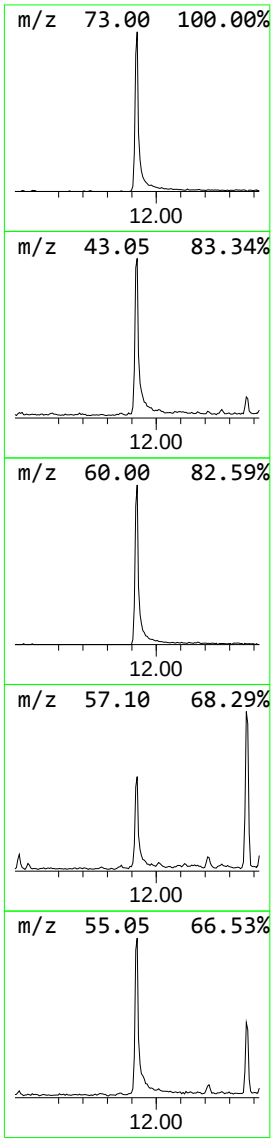
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	8.19 ng	972578	Phenanthrene-d10	11.386

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	95
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

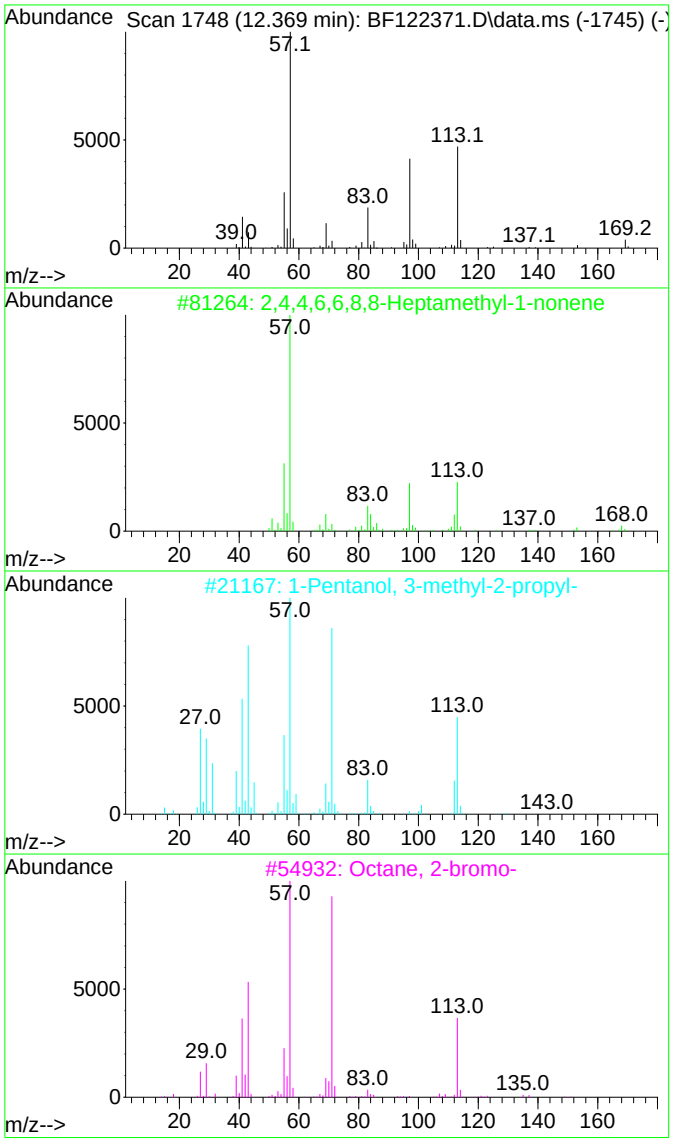
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

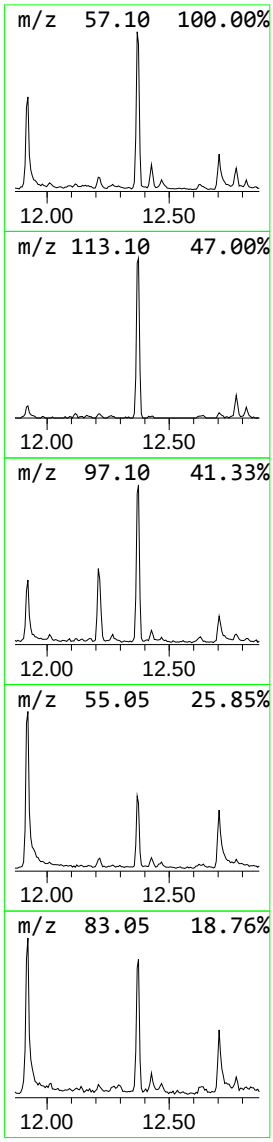
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.368	2.20 ng	260878	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	56
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	38
4	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	32
5	Octane, 2-iodo-	240	C8H17I	000557-36-8	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

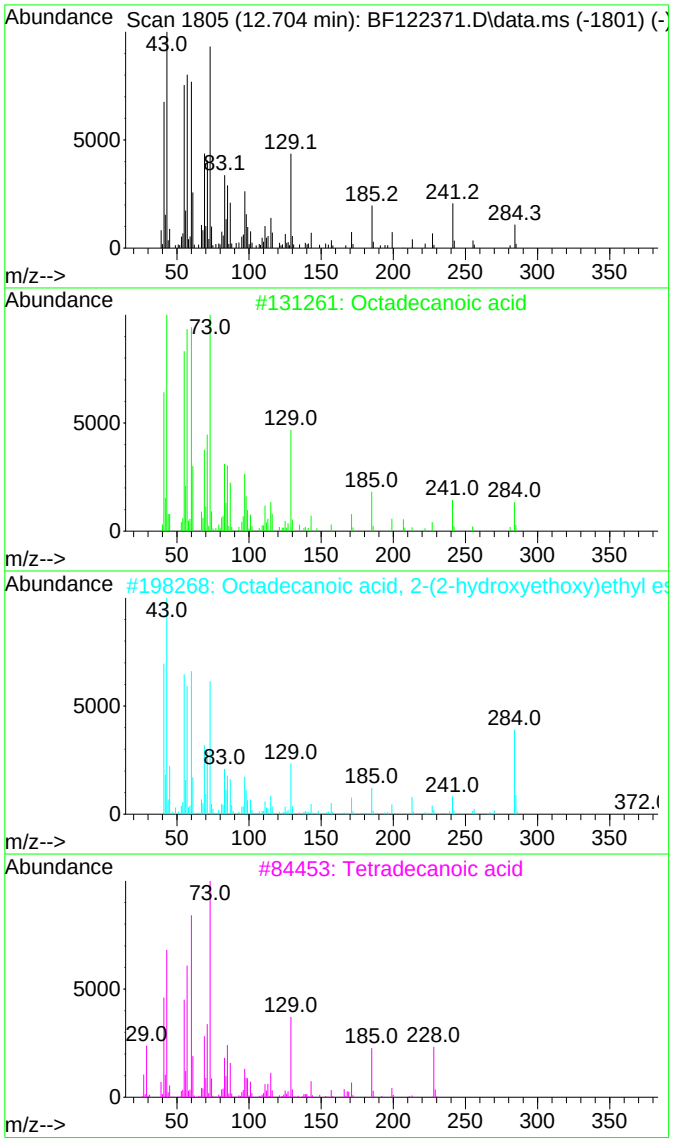
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

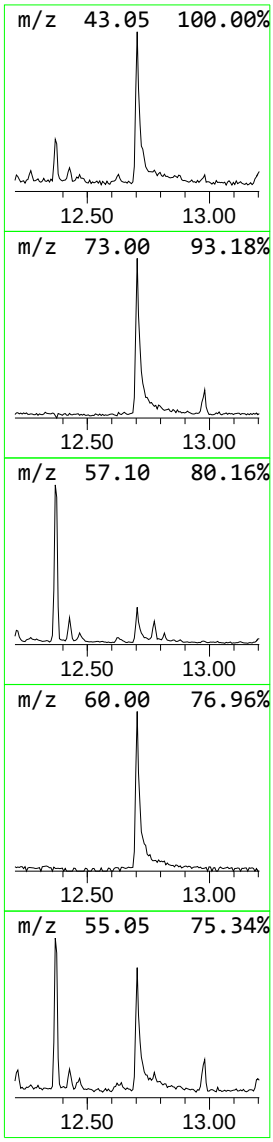
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	3.28 ng	388971	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

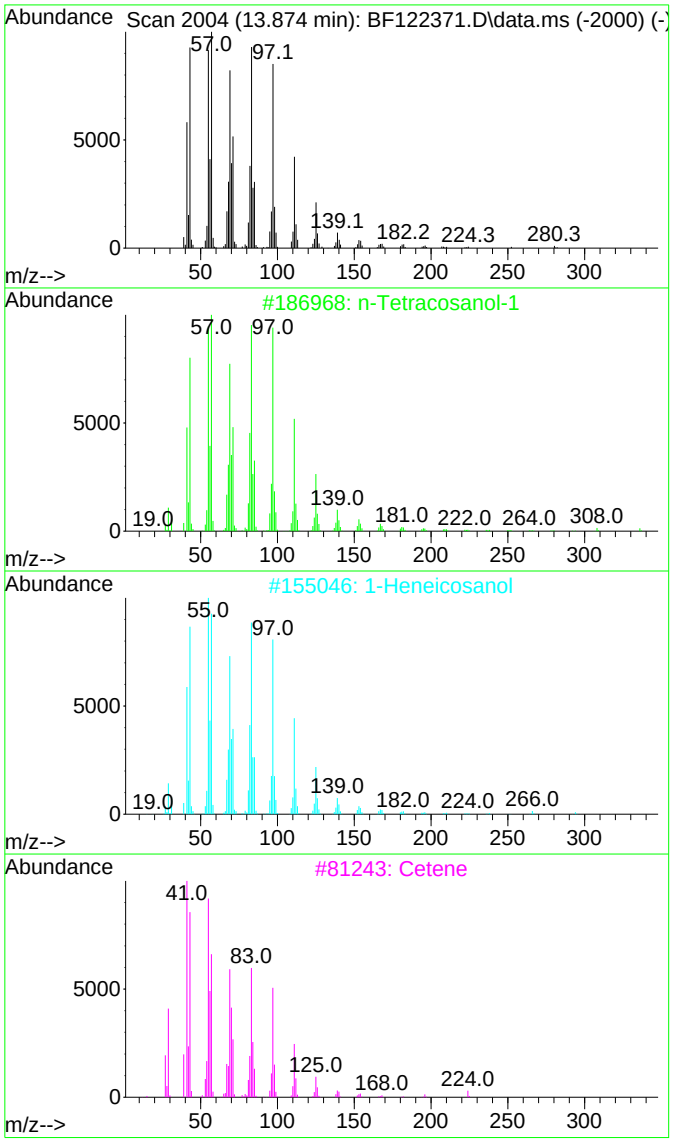
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

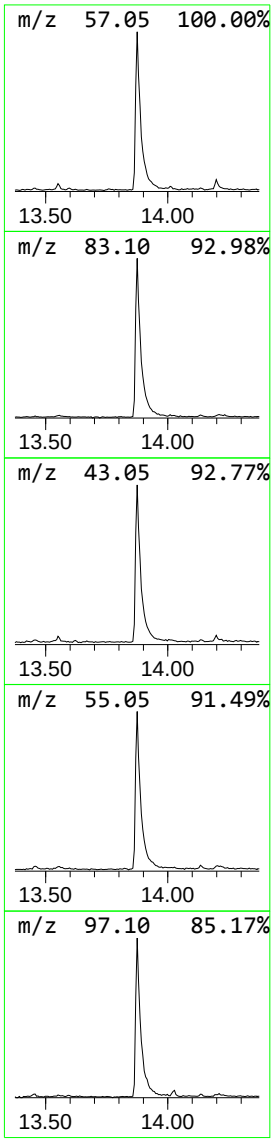
****

Peak Number 8 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	11.64 ng	1474170	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Cetene	224	C16H32	000629-73-2	95
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

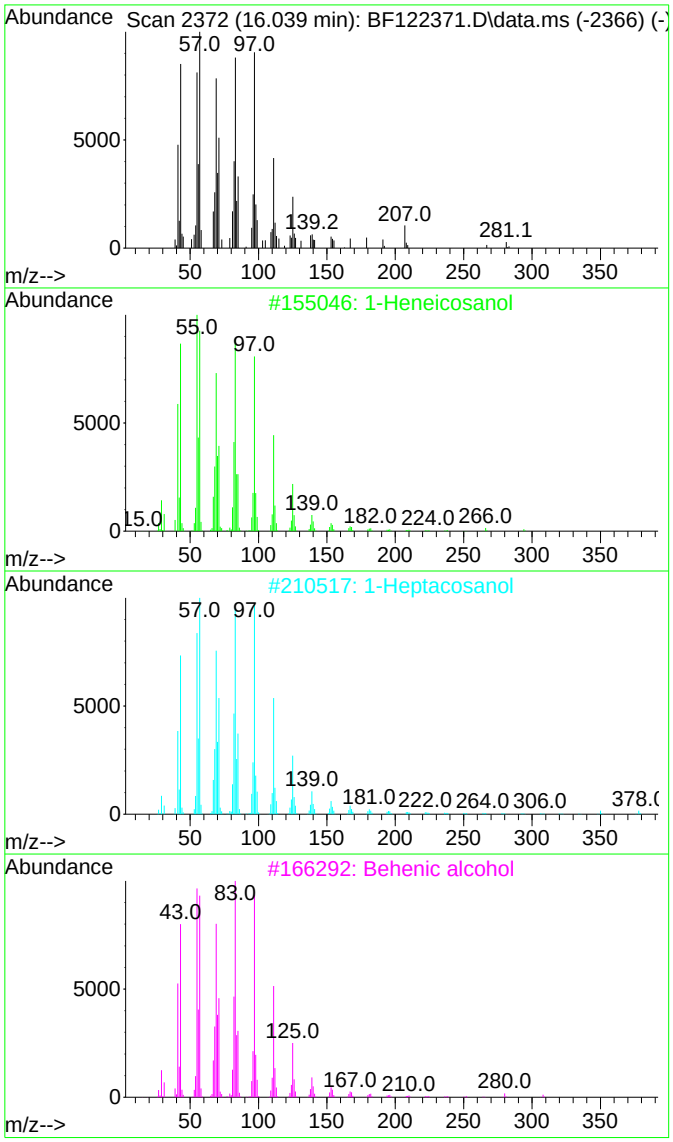
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

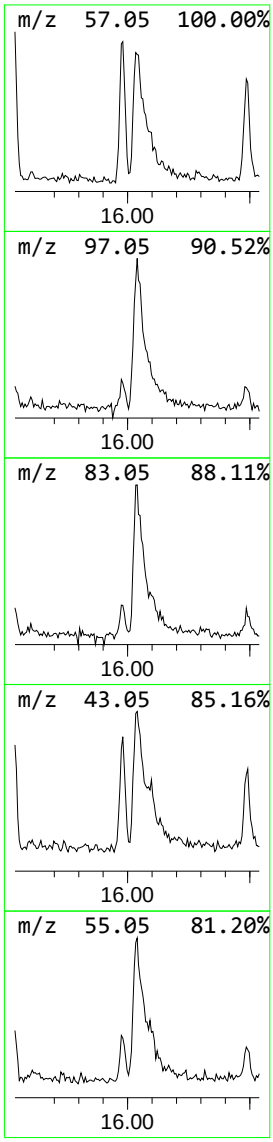
****

Peak Number 9 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	2.51 ng	297431	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	1-Nonadecene	266	C19H38	018435-45-5	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122371.D
Acq On : 18 Nov 2020 17:00
Operator : JU/CG
Sample : L4771-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-02-2-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Butane, 2-metho...	2.152	18.1	ng	1254880	1	6.863	1387840	20.0
3-Penten-2-one,...	4.457	14.5	ng	1004440	1	6.863	1387840	20.0
2-Pentanone, 4-...	5.081	6.0	ng	416480	1	6.863	1387840	20.0
Ethanol, 2-(2-e...	6.687	2.1	ng	145682	1	6.863	1387840	20.0
n-Hexadecanoic ...	11.922	8.2	ng	972578	4	11.386	2373800	20.0
2,4,4,6,6,8,8-H...	12.368	2.2	ng	260878	4	11.386	2373800	20.0
Octadecanoic acid	12.704	3.3	ng	388971	4	11.386	2373800	20.0
n-Tetracosanol-1	13.874	11.6	ng	1474170	5	14.027	2532870	20.0
1-Heneicosanol	16.039	2.5	ng	297431	6	15.498	2366670	20.0