LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
Data File : BF129382.D
Acq On : 27 Jul 2022 18:17
Operator : CG\JU
Sample : N3861-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB-072122

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129382.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	478	480	491	rVB	202398	223961	2.61%	0.487%
2	5.504	543	547	551	rVB	3396896	3090194	36.03%	6.713%
3	6.504	713	717	729	rVB	2056127	1915513	22.33%	4.161%
4	6.881	777	781	785	rBV	1809319	1463367	17.06%	3.179%
5	6.939	787	791	801	rBV	75084	92729	1.08%	0.201%
6	7.451	868	878	881	rBV	4565218	5037413	58.73%	10.943%
7	7.528	886	891	899	rVB3	52802	87820	1.02%	0.191%
8	7.686	910	918	929	rBV3	180387	412743	4.81%	0.897%
9	8.163	994	999	1002	rBV	2220557	1959377	22.84%	4.256%
10	8.375	1031	1035	1037	rBV	481658	451768	5.27%	0.981%
11	8.404	1037	1040	1051	rVB	630675	698348	8.14%	1.517%
12	9.245	1176	1183	1186	rBV	8191707	8577757	100.00%	18.633%
13	9.351	1197	1201	1205	rBV	125826	113399	1.32%	0.246%
14	9.922	1292	1298	1301	rBV	2696963	2234246	26.05%	4.853%
15	10.716	1426	1433	1436	rBV	5500759	5603959	65.33%	12.173%
16	11.410	1546	1551	1555	rBV	2326261	2172076	25.32%	4.718%
17	11.792	1613	1616	1620	rVB	358556	271156	3.16%	0.589%
18	13.004	1816	1822	1825	rBV	8152262	8415351	98.11%	18.280%
19	13.915	1970	1977	1987	rBV5	54343	179066	2.09%	0.389%
20	14.057	1997	2001	2005	rBV	1871224	1620550	18.89%	3.520%
21	14.898	2140	2144	2149	rBV	171694	171228	2.00%	0.372%
22	15.545	2249	2254	2266	rBV2	975995	1242783	14.49%	2.700%

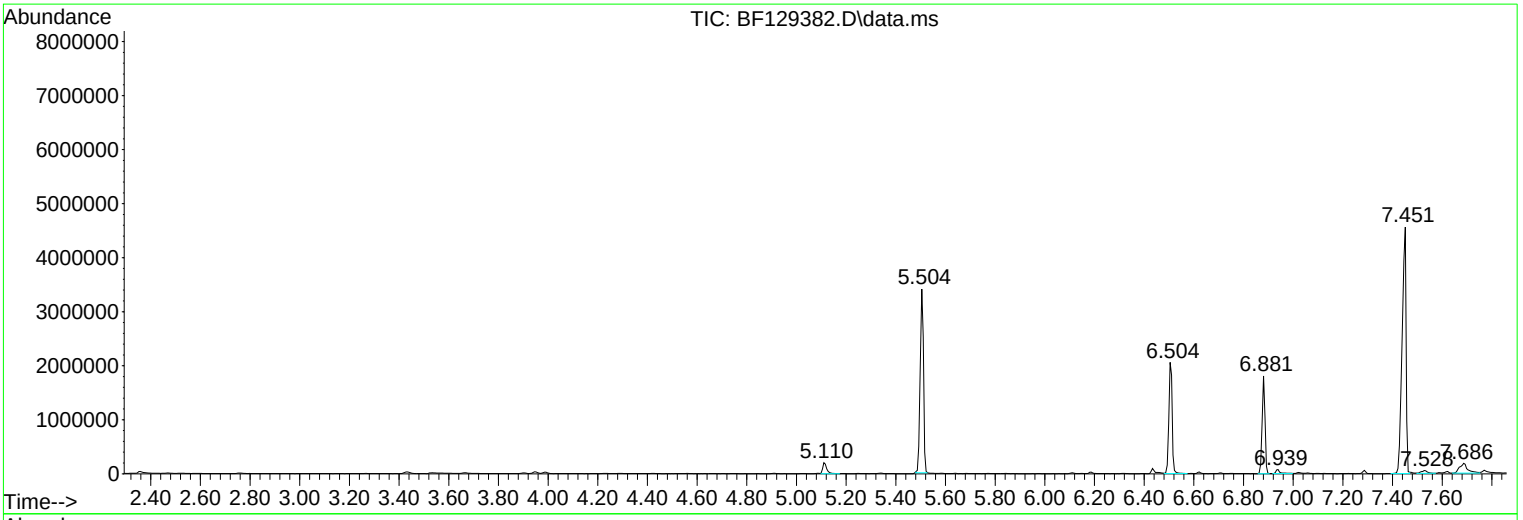
Sum of corrected areas: 46034804

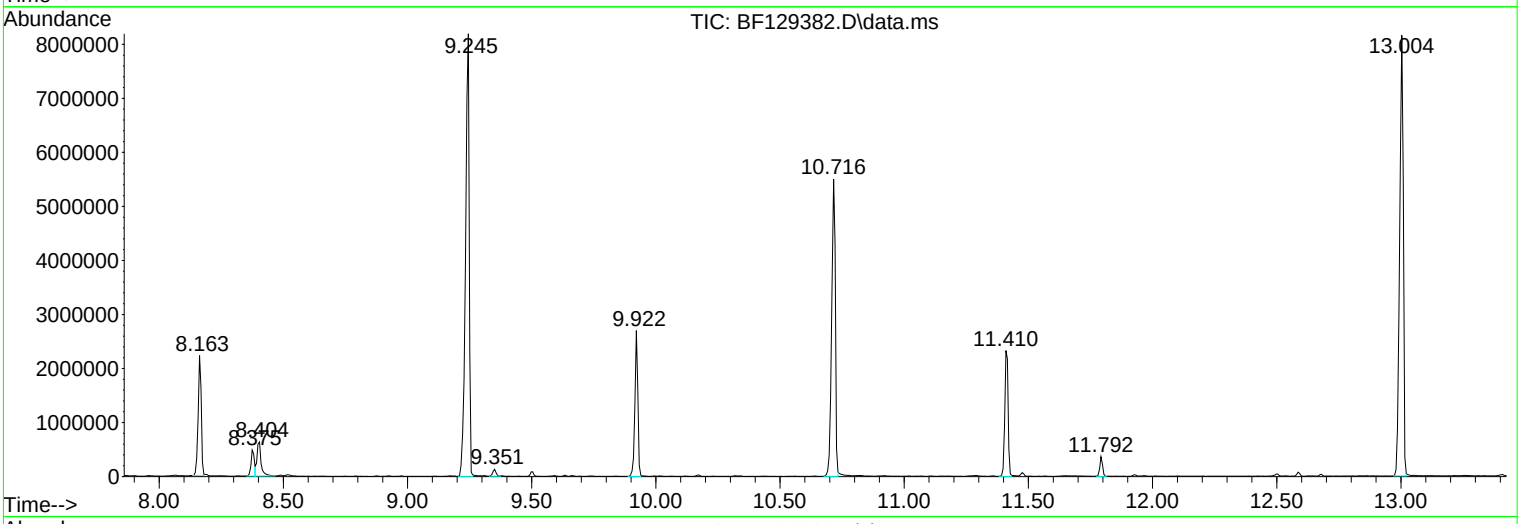
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
Data File : BF129382.D
Acq On : 27 Jul 2022 18:17
Operator : CG\JU
Sample : N3861-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

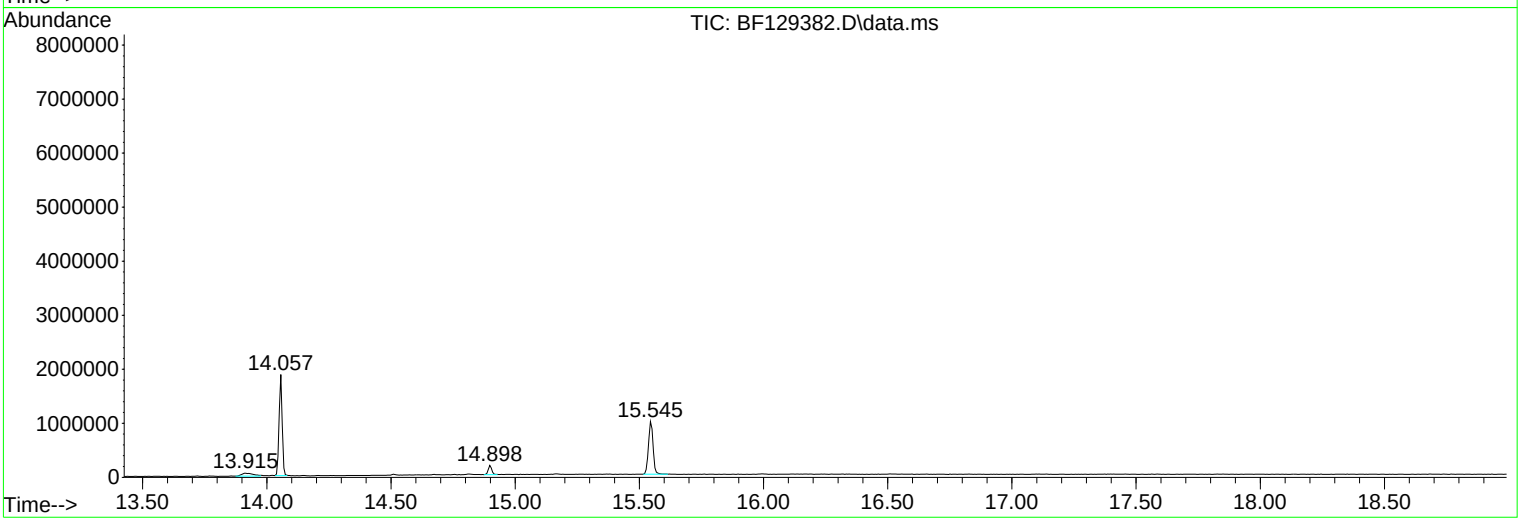
Instrument :
BNA_F
ClientSampleId :
FB-072122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
Data File : BF129382.D
Acq On : 27 Jul 2022 18:17
Operator : CG\JU
Sample : N3861-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-072122

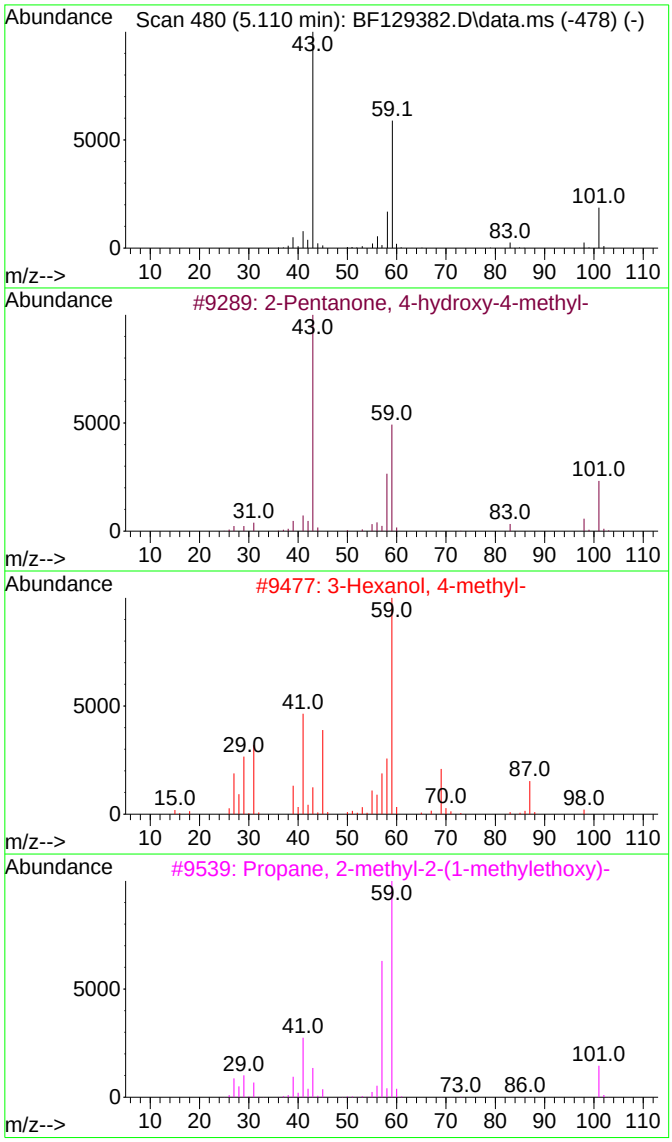
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

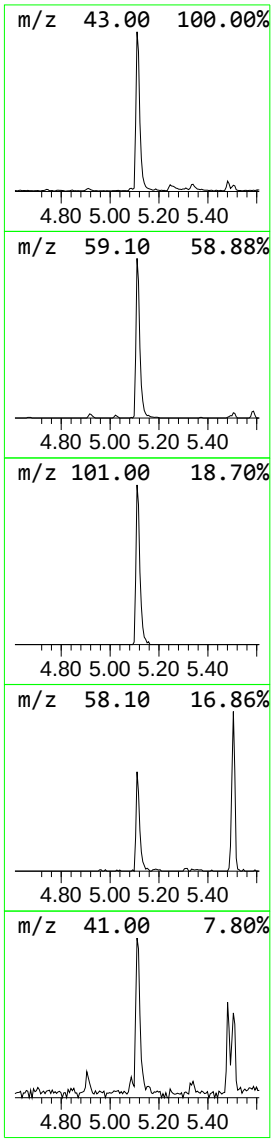
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	3.06 ng	223961	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
Data File : BF129382.D
Acq On : 27 Jul 2022 18:17
Operator : CG\JU
Sample : N3861-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-072122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

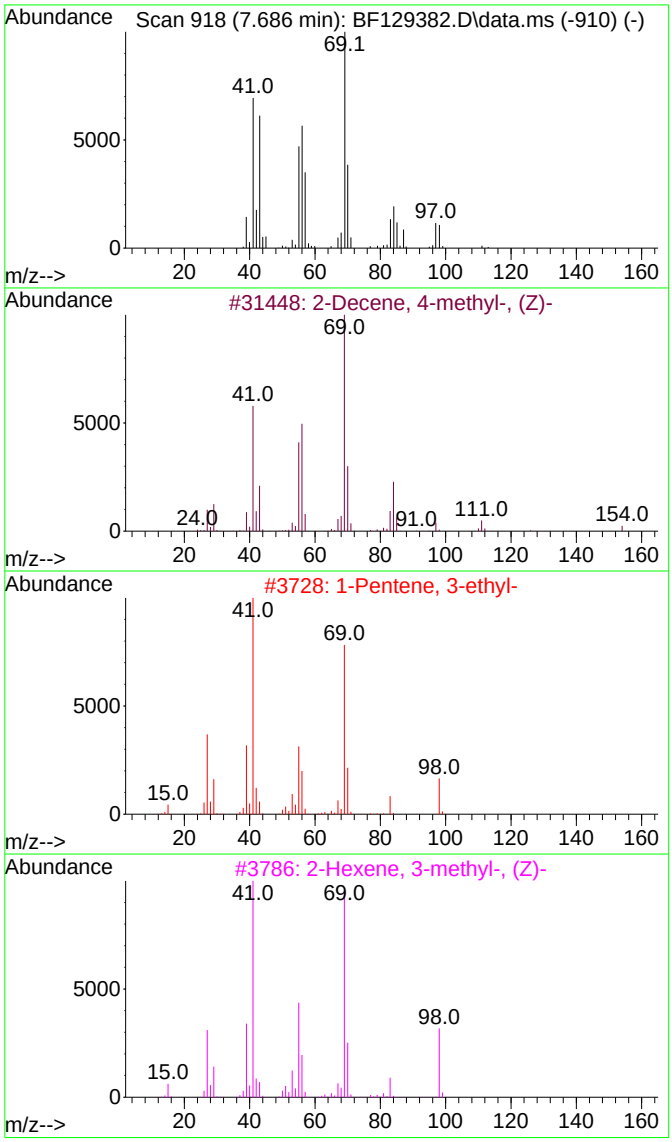
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

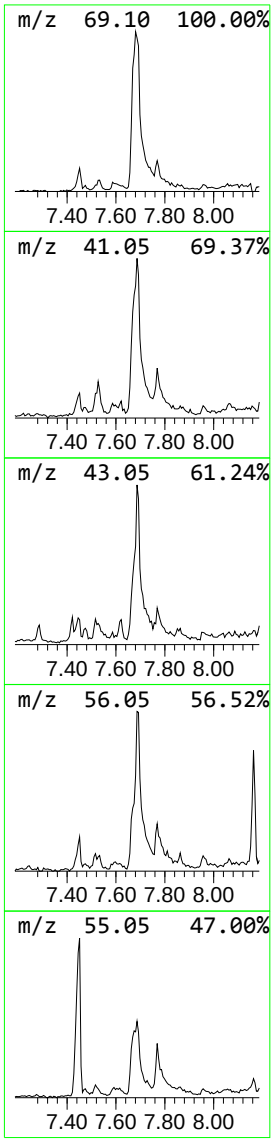
****

Peak Number 2 2-Decene, 4-methyl-, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.686	4.21 ng	412743	Naphthalene-d8	8.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decene, 4-methyl-, (Z)-	154	C11H22	074630-30-1	72
2	1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	58
3	2-Hexene, 3-methyl-, (Z)-	98	C7H14	010574-36-4	53
4	3-Methyl-2-hexene	98	C7H14	017618-77-8	50
5	Cyclopropanecarboxylic acid, 2-e...	198	C12H22O2	103604-31-5	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
Data File : BF129382.D
Acq On : 27 Jul 2022 18:17
Operator : CG\JU
Sample : N3861-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-072122

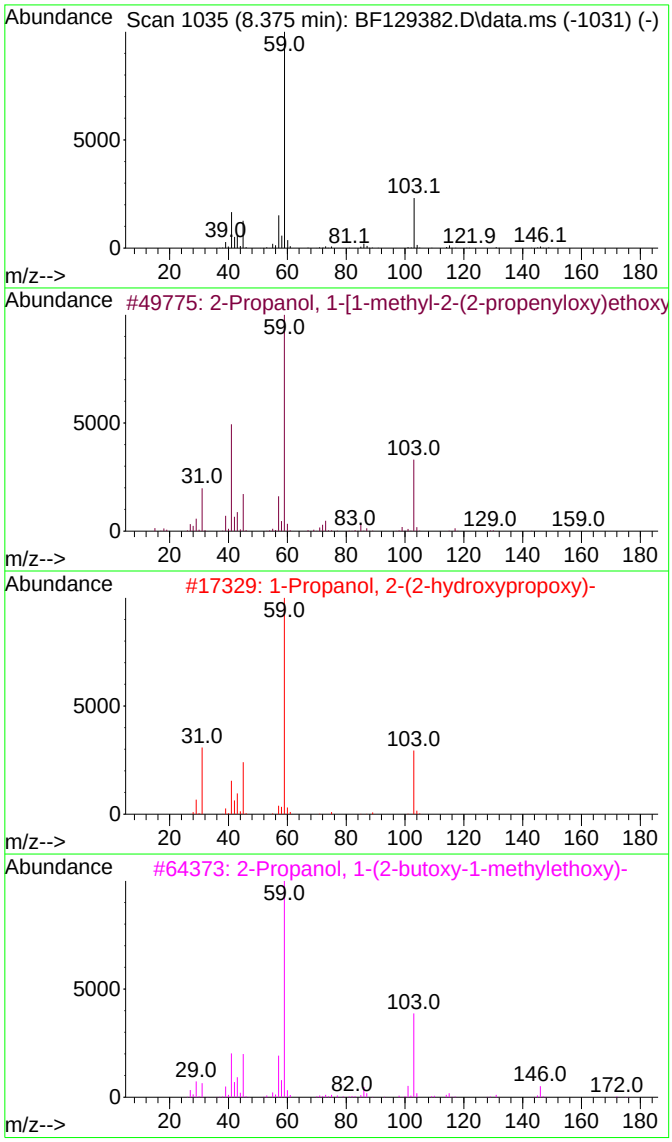
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

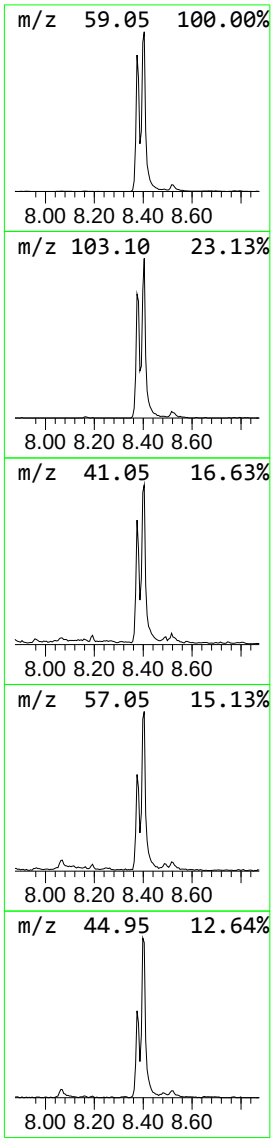
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.375	4.61 ng	451768	Naphthalene-d8	8.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	83
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
3	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	74
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	72
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
Data File : BF129382.D
Acq On : 27 Jul 2022 18:17
Operator : CG\JU
Sample : N3861-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-072122

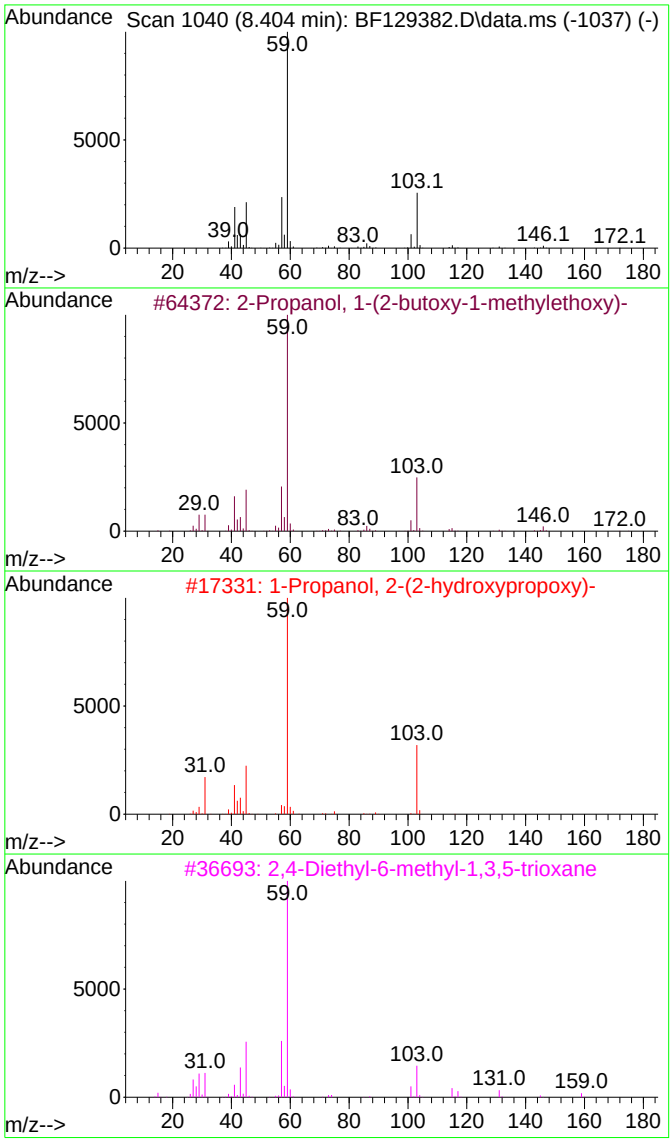
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

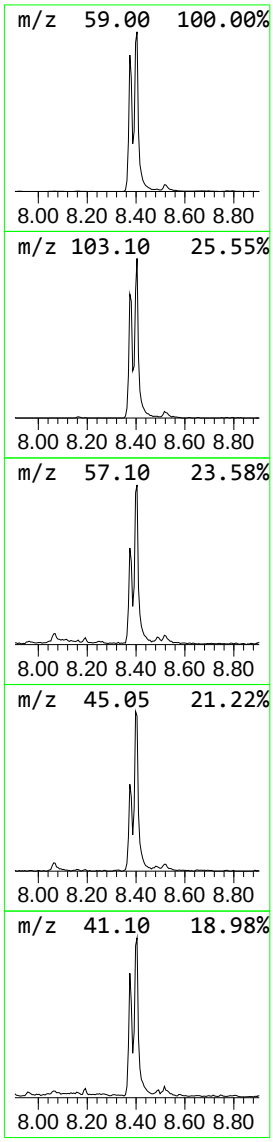
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.404	7.13 ng	698348	Naphthalene-d8	8.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	90
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
3	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	78
4	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	64
5	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
Data File : BF129382.D
Acq On : 27 Jul 2022 18:17
Operator : CG\JU
Sample : N3861-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-072122

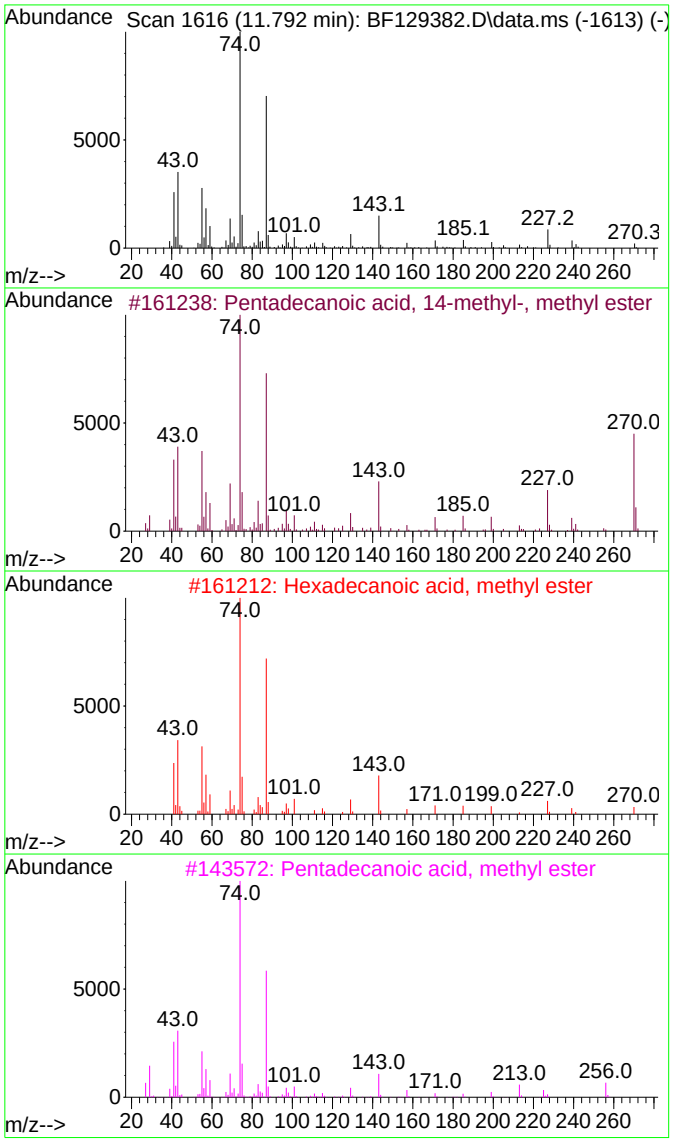
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

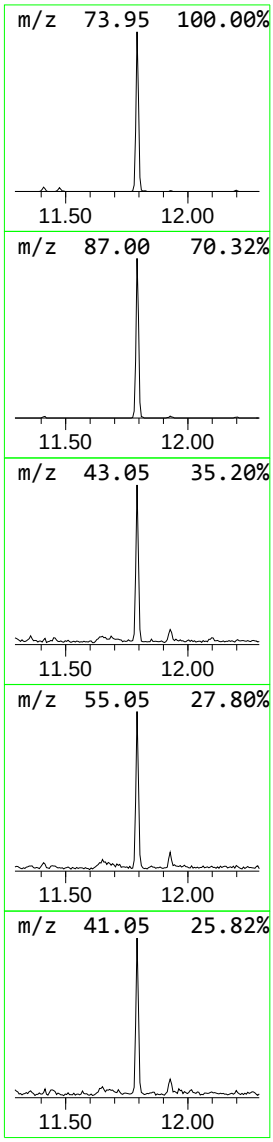
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentadecanoic acid, 14-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	2.50 ng	271156	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
Data File : BF129382.D
Acq On : 27 Jul 2022 18:17
Operator : CG\JU
Sample : N3861-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-072122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

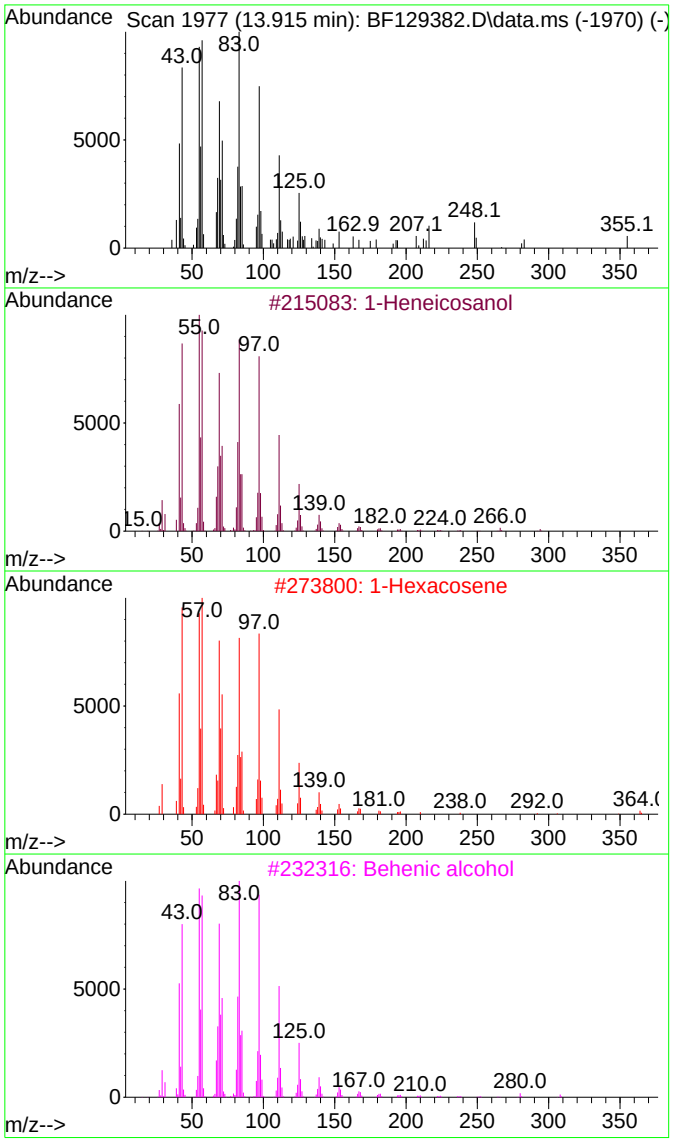
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

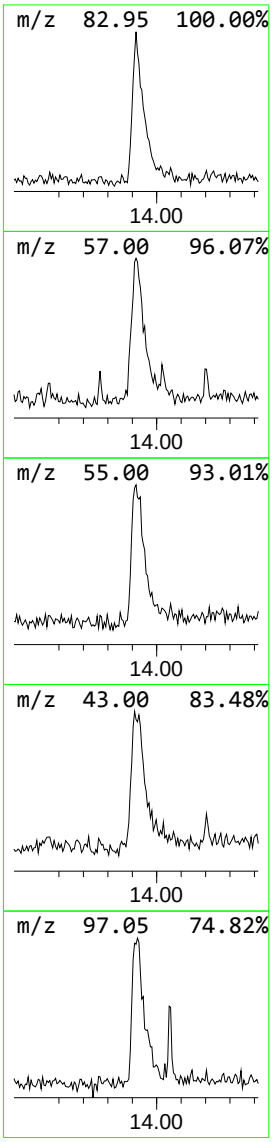
****

Peak Number 6 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.915	2.21 ng	179066	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
Data File : BF129382.D
Acq On : 27 Jul 2022 18:17
Operator : CG\JU
Sample : N3861-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-072122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

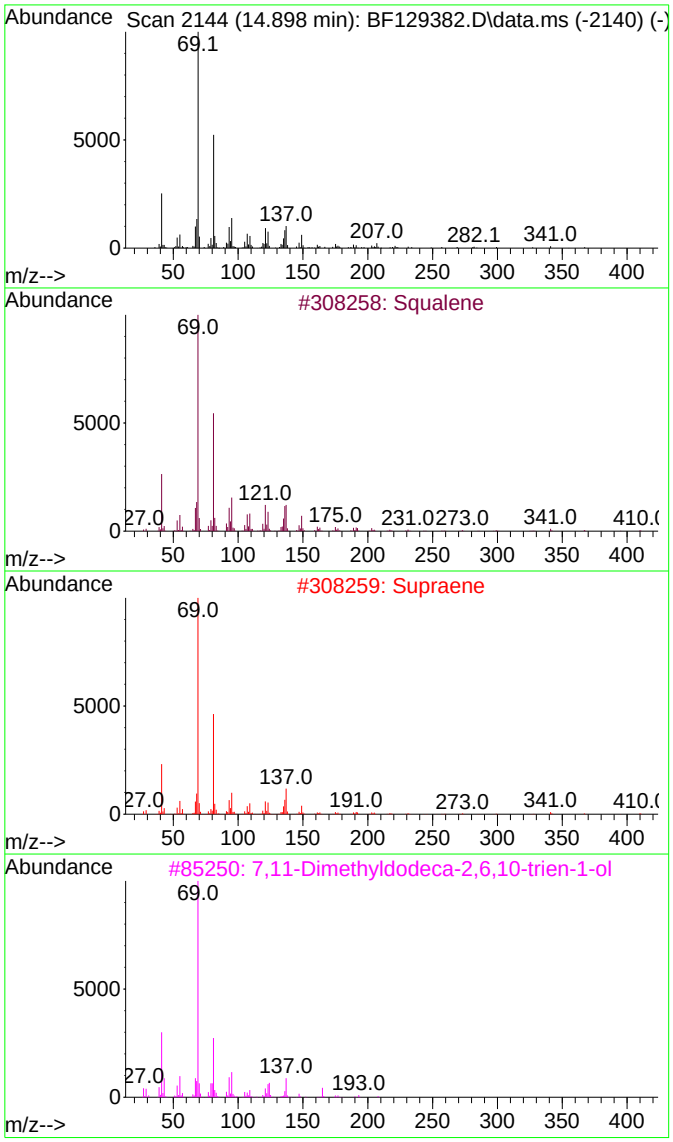
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

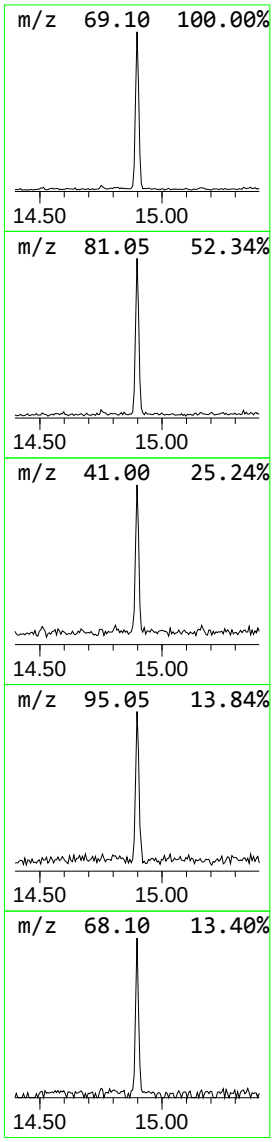
****

Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	2.76 ng	171228	Perylene-d12	15.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	87
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	83
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
Data File : BF129382.D
Acq On : 27 Jul 2022 18:17
Operator : CG\JU
Sample : N3861-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-072122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.110	3.1	ng	223961	1	6.881	1463370	20.0
2-Decene, 4-met...	7.686	4.2	ng	412743	2	8.163	1959380	20.0
2-Propanol, 1-[...	8.375	4.6	ng	451768	2	8.163	1959380	20.0
2-Propanol, 1-(...	8.404	7.1	ng	698348	2	8.163	1959380	20.0
Pentadecanoic a...	11.792	2.5	ng	271156	4	11.410	2172080	20.0
1-Heneicosanol	13.915	2.2	ng	179066	5	14.057	1620550	20.0
Squalene	14.898	2.8	ng	171228	6	15.545	1242780	20.0