LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124046.D
Acq On : 24 May 2021 19:50
Operator : JU/CG
Sample : M2479-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUBBASE-6-1-D

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124046.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	13	rBV	360905	433125	38.68%	4.940%
2	2.240	22	26	30	rBV	31073	38197	3.41%	0.436%
3	5.104	509	513	519	rVB	165968	177530	15.85%	2.025%
4	5.510	578	582	595	rBV	1187434	1093598	97.66%	12.472%
5	5.904	647	649	654	rVB	17816	15802	1.41%	0.180%
6	6.522	749	754	757	rBV	1187109	1069474	95.50%	12.197%
7	6.722	785	788	792	rBV2	15857	16867	1.51%	0.192%
8	6.893	814	817	821	rBV	373178	310333	27.71%	3.539%
9	7.457	908	913	916	rBV	799737	680079	60.73%	7.756%
10	8.181	1032	1036	1039	rVB	400088	333279	29.76%	3.801%
11	9.198	1207	1209	1212	rVB2	30095	26788	2.39%	0.305%
12	9.251	1215	1218	1221	rBV	1369413	1119811	100.00%	12.771%
13	9.334	1229	1232	1235	rBV4	23165	25726	2.30%	0.293%
14	9.369	1235	1238	1240	rVB2	56812	48768	4.36%	0.556%
15	9.645	1282	1285	1289	rBV	201552	192969	17.23%	2.201%
16	9.745	1298	1302	1307	rVB7	11746	24160	2.16%	0.276%
17	9.804	1307	1312	1314	rBV5	21415	26213	2.34%	0.299%
18	9.845	1317	1319	1322	rVB3	21584	20592	1.84%	0.235%
19	9.934	1331	1334	1338	rVB	479446	371003	33.13%	4.231%
20	10.345	1401	1404	1409	rVB6	16043	20524	1.83%	0.234%
21	10.581	1441	1444	1450	rVB5	22694	31525	2.82%	0.360%
22	10.628	1450	1452	1456	rBV5	9082	14412	1.29%	0.164%
23	10.722	1464	1468	1472	rBV	871763	733494	65.50%	8.365%
24	10.851	1486	1490	1493	rVB	77230	73160	6.53%	0.834%
25	10.922	1500	1502	1506	rVB5	16953	19733	1.76%	0.225%
26	11.163	1539	1543	1544	rBV2	12279	14028	1.25%	0.160%
27	11.316	1566	1569	1575	rVB	46211	55421	4.95%	0.632%
28	11.422	1584	1587	1591	rVB	433996	370368	33.07%	4.224%
29	11.663	1626	1628	1632	rVB4	13697	15600	1.39%	0.178%
30	11.816	1650	1654	1656	rBV5	12474	14439	1.29%	0.165%
31	11.945	1673	1676	1679	rBV4	53897	50332	4.49%	0.574%
32	13.010	1853	1857	1861	rBV	1118154	991124	88.51%	11.303%
33	13.916	2009	2011	2016	rBV3	104711	126233	11.27%	1.440%
34	14.069	2034	2037	2040	rBV	246874	213890	19.10%	2.439%

Sum of corrected areas: 8768597

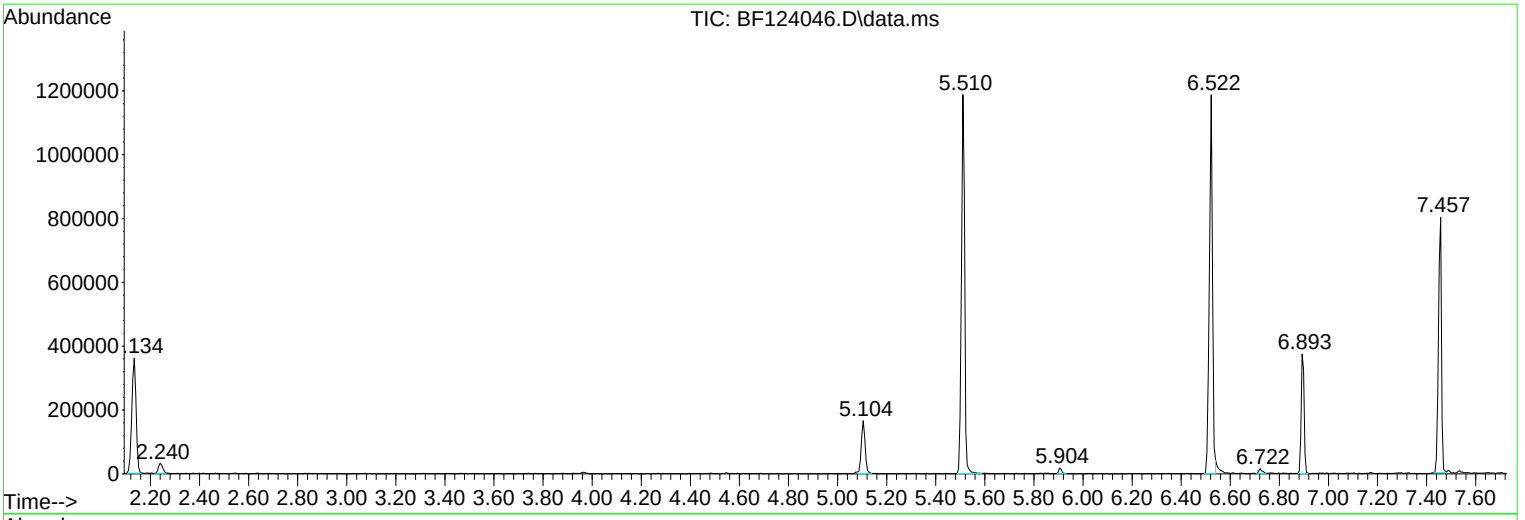
Instrument :
BNA_F
ClientSampleId :
SUBBASE-6-1-D

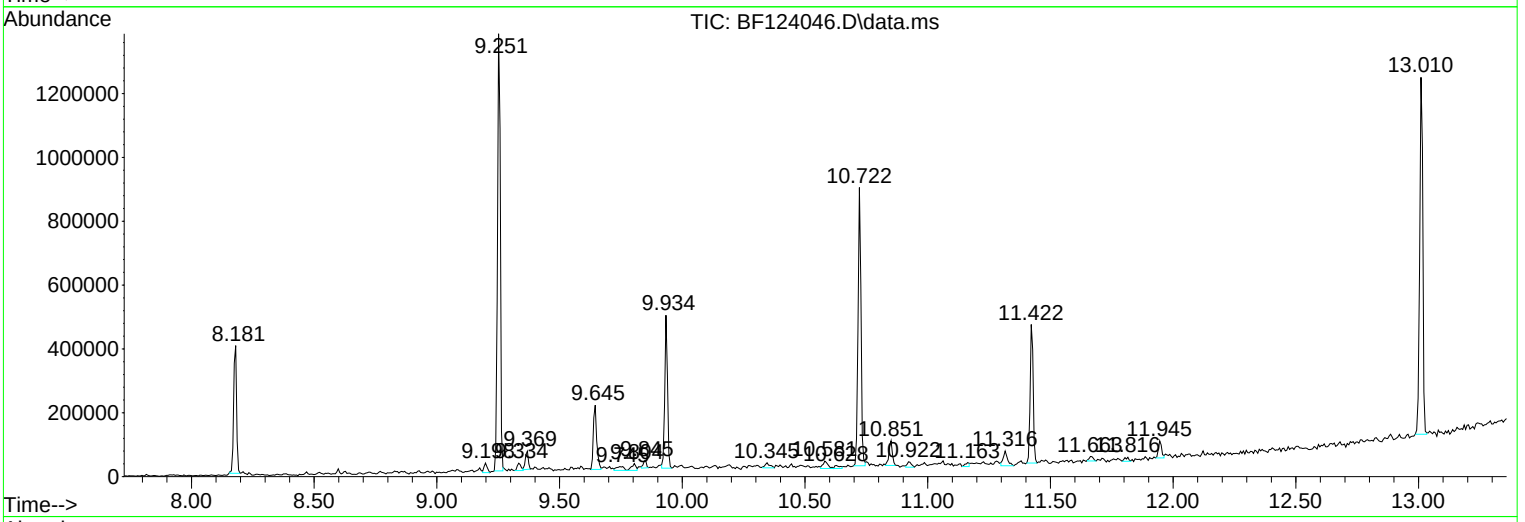
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124046.D
Acq On : 24 May 2021 19:50
Operator : JU/CG
Sample : M2479-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

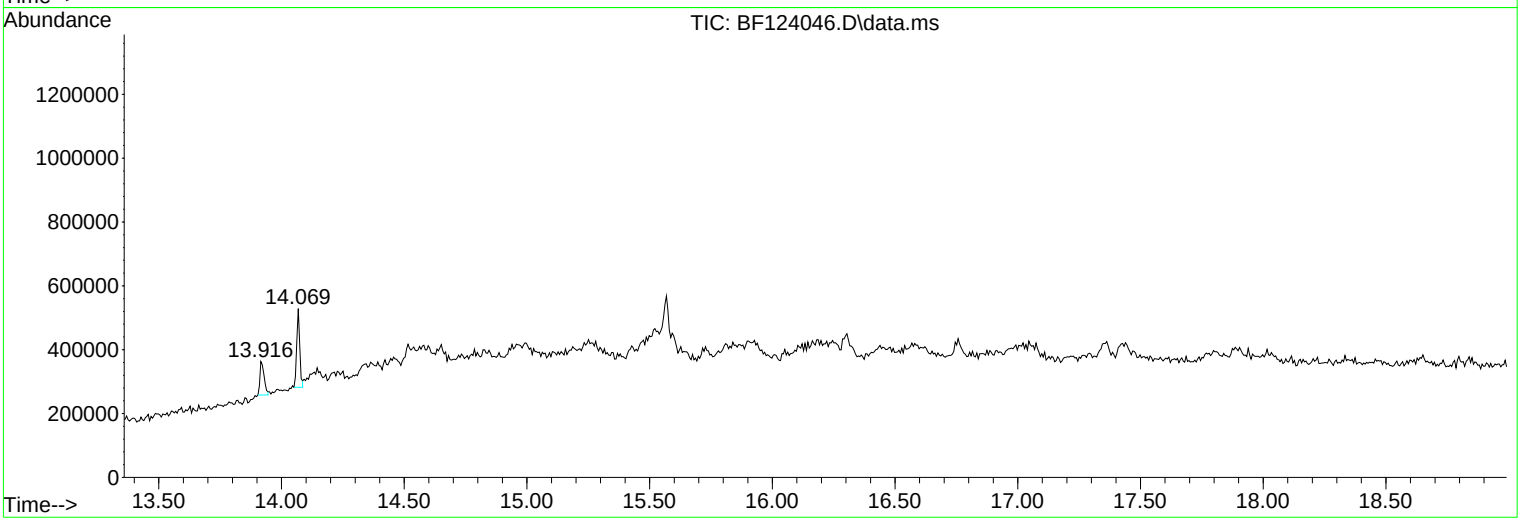
Instrument :
BNA_F
ClientSampleId :
SUBBASE-6-1-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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Data File : BF124046.D
Acq On : 24 May 2021 19:50
Operator : JU/CG
Sample : M2479-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
SUBBASE-6-1-D

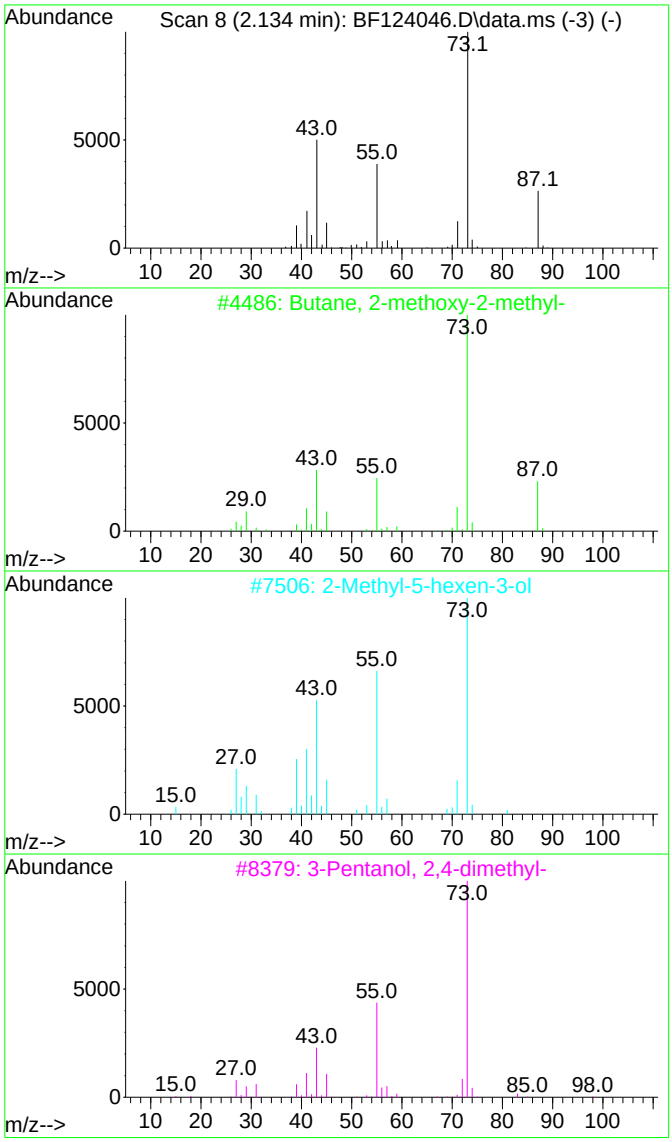
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

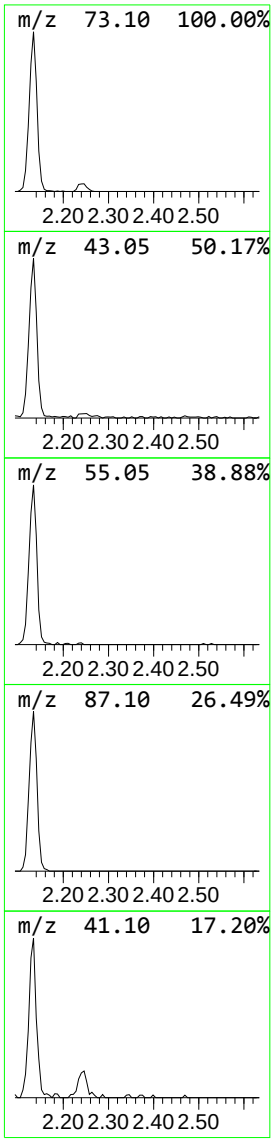
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	27.91 ng	433125	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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Data File : BF124046.D
Acq On : 24 May 2021 19:50
Operator : JU/CG
Sample : M2479-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUBBASE-6-1-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

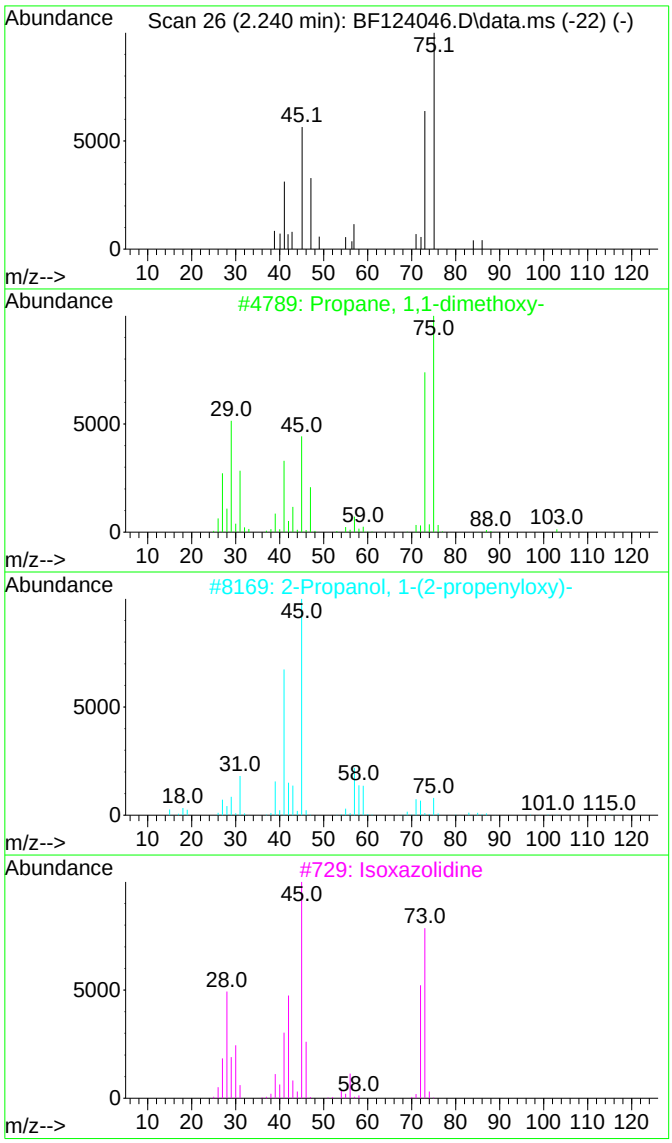
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

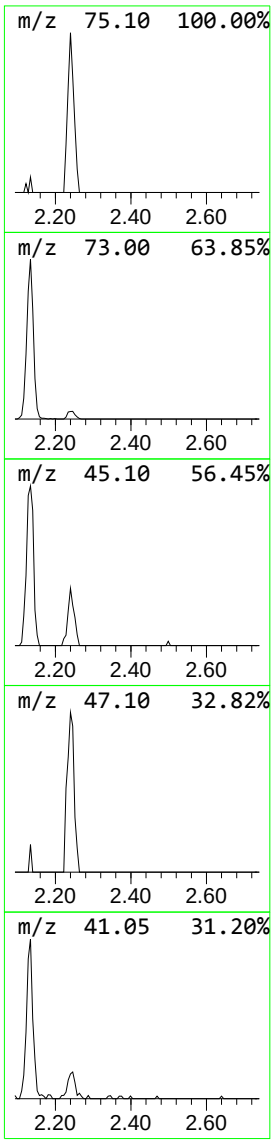
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	2.46 ng	38197	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	2-Propanol, 1-(2-propenyloxy)-	116	C6H12O2	021460-36-6	9
3	Isoxazolidine	73	C3H7NO	000504-72-3	4
4	Glycine	75	C2H5NO2	000056-40-6	4
5	Methane, nitroso-	45	CH3NO	000865-40-7	4





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Data File : BF124046.D
Acq On : 24 May 2021 19:50
Operator : JU/CG
Sample : M2479-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUBBASE-6-1-D

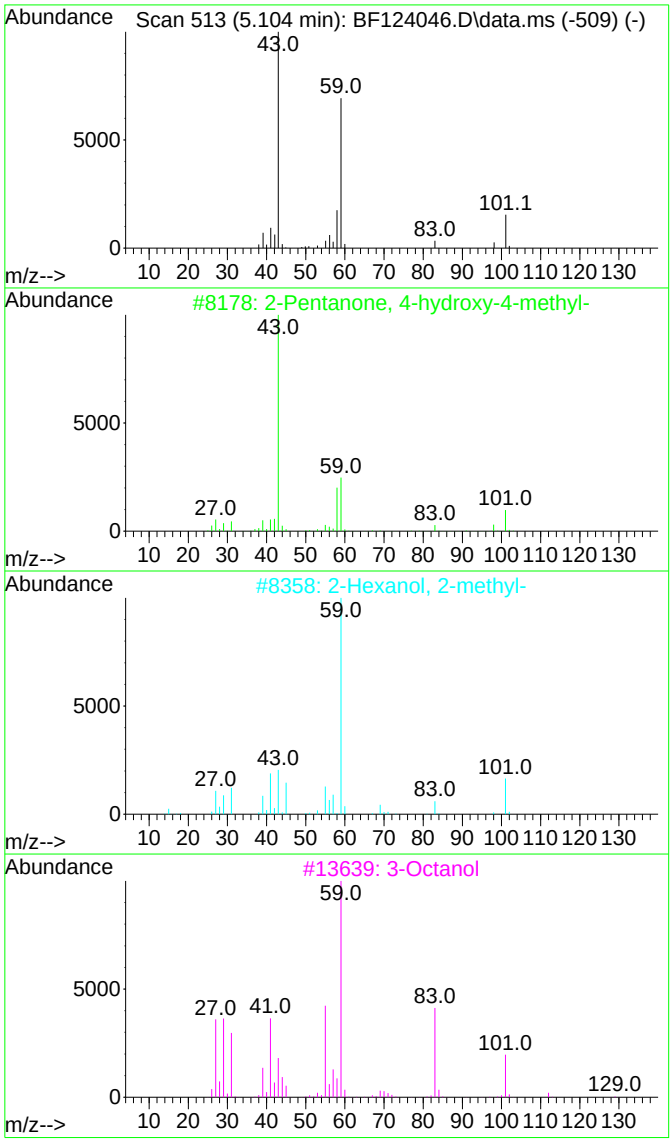
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

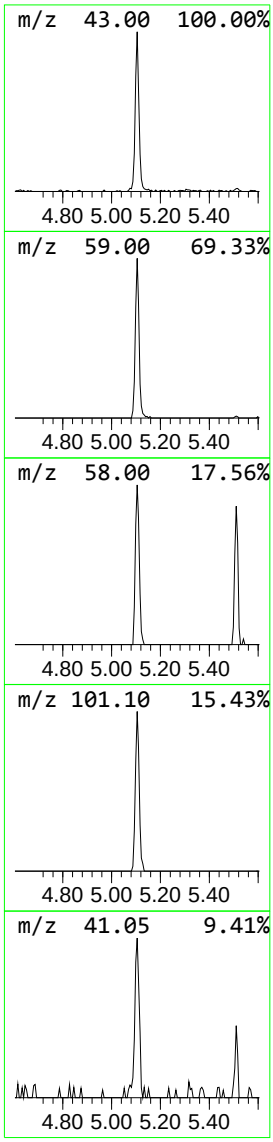
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	11.44 ng	177530	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	42
3	3-Octanol	130	C8H18O	000589-98-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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Operator : JU/CG
Sample : M2479-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUBBASE-6-1-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

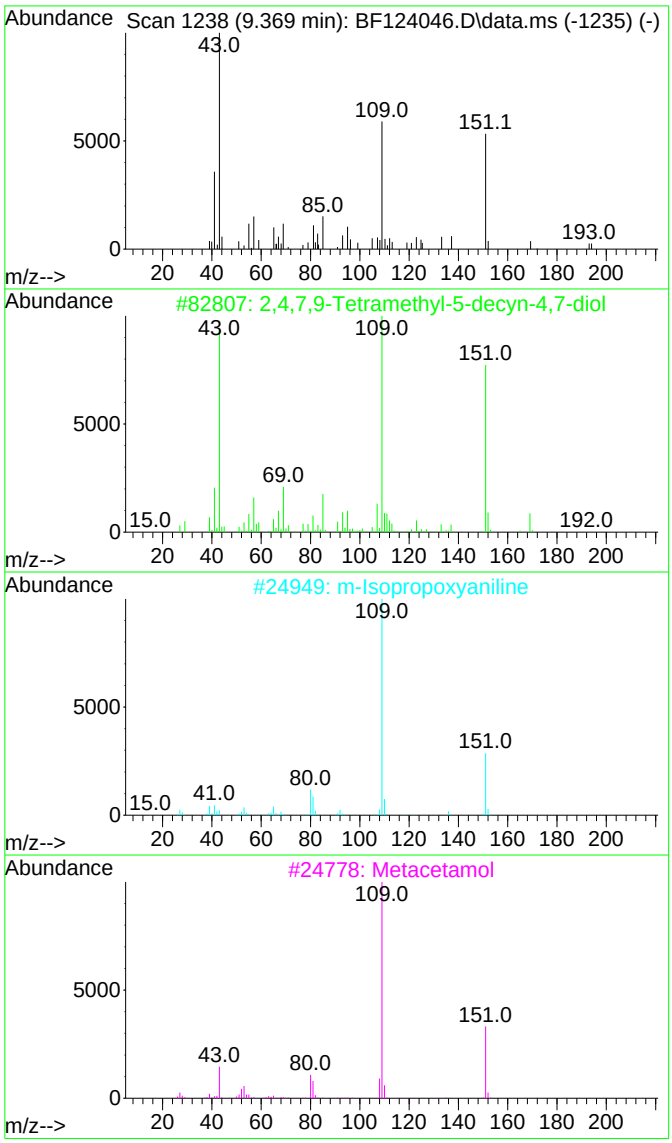
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

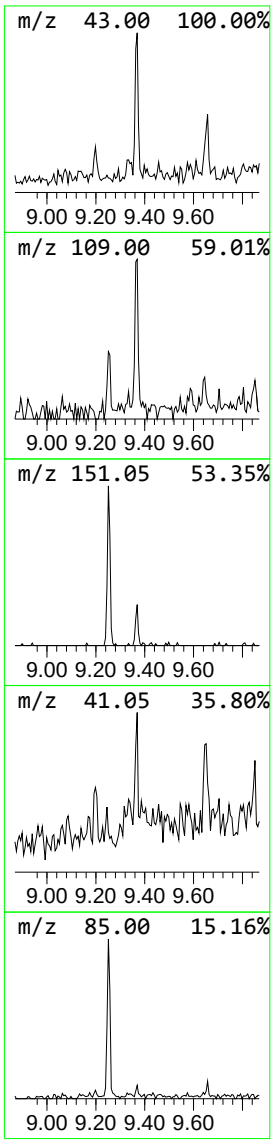
****

Peak Number 4 unknown9.369 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.369	2.63 ng	48768	Acenaphthene-d10	9.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	42
2	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	40
3	Metacetamol	151	C8H9NO2	000621-42-1	40
4	(7,7-Dimethyl-2-oxobicyclo[2.2.1...	250	C10H15ClO3S	1000194-76-1	38
5	2-Cyclohexen-1-ol, 2-methyl-5-(1...	152	C10H16O	001197-06-4	35





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Sample : M2479-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
SUBBASE-6-1-D

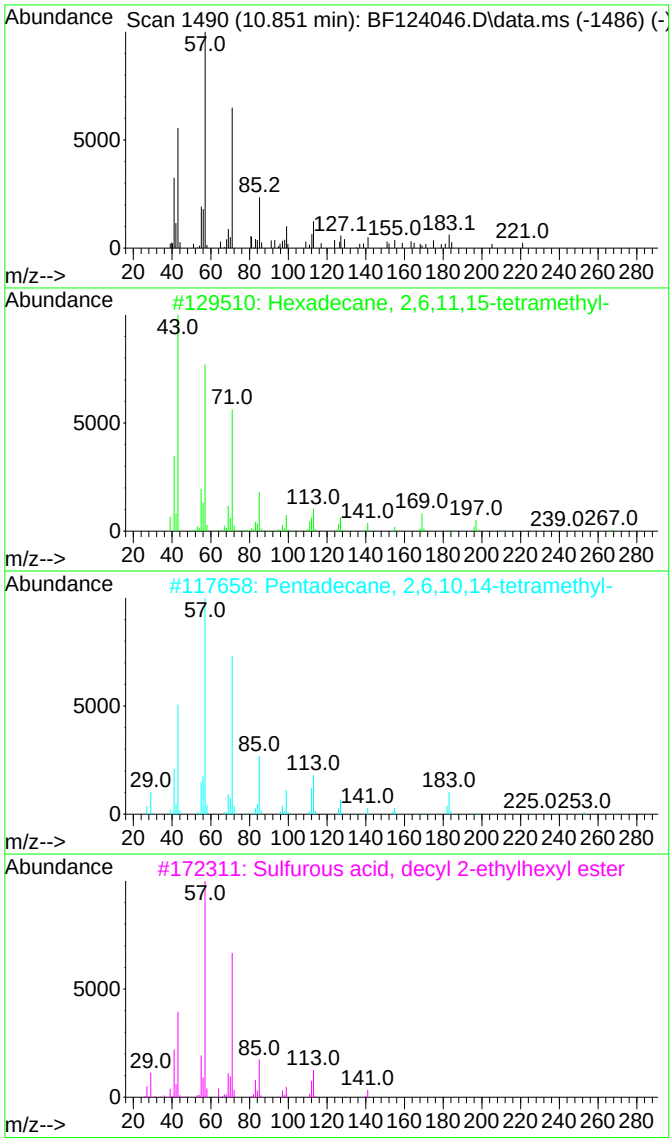
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

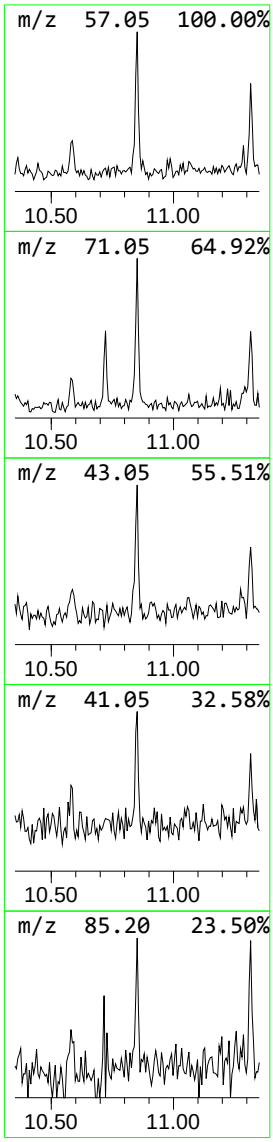
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexadecane, 2,6,11,15-tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	3.95 ng	73160	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	78
2	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	72
3	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	72
4	Tridecane	184	C13H28	000629-50-5	64
5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64





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Operator : JU/CG
Sample : M2479-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUBBASE-6-1-D

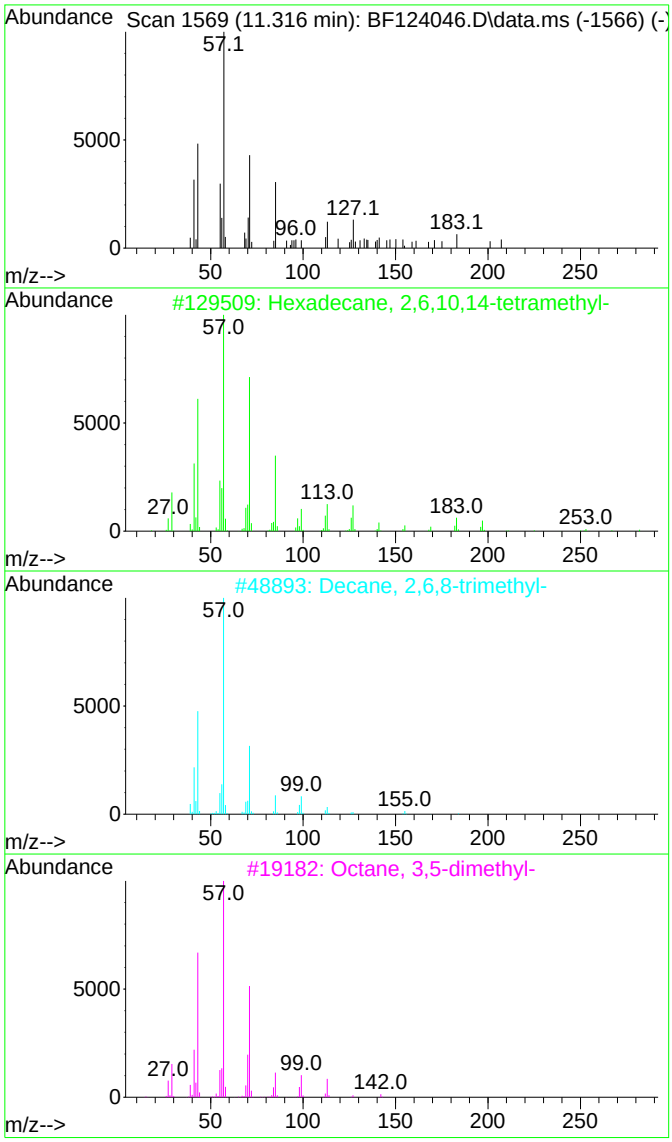
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

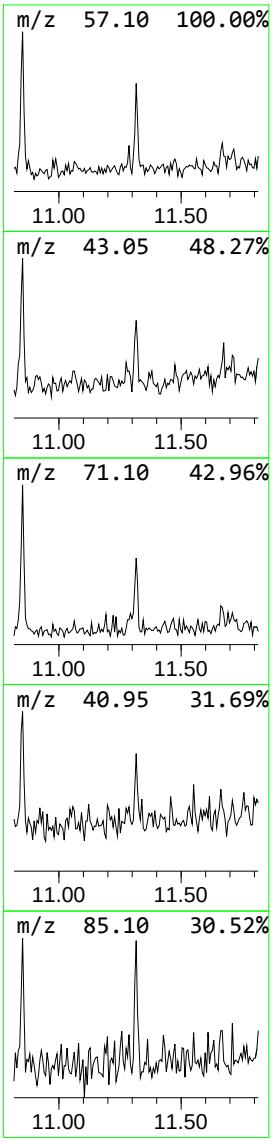
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexadecane, 2,6,10,14-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.316	2.99 ng	55421	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	59
2	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	50
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	47
4	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	47
5	9-methylheptadecane	254	C18H38	026741-18-4	47





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Data File : BF124046.D
Acq On : 24 May 2021 19:50
Operator : JU/CG
Sample : M2479-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUBBASE-6-1-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

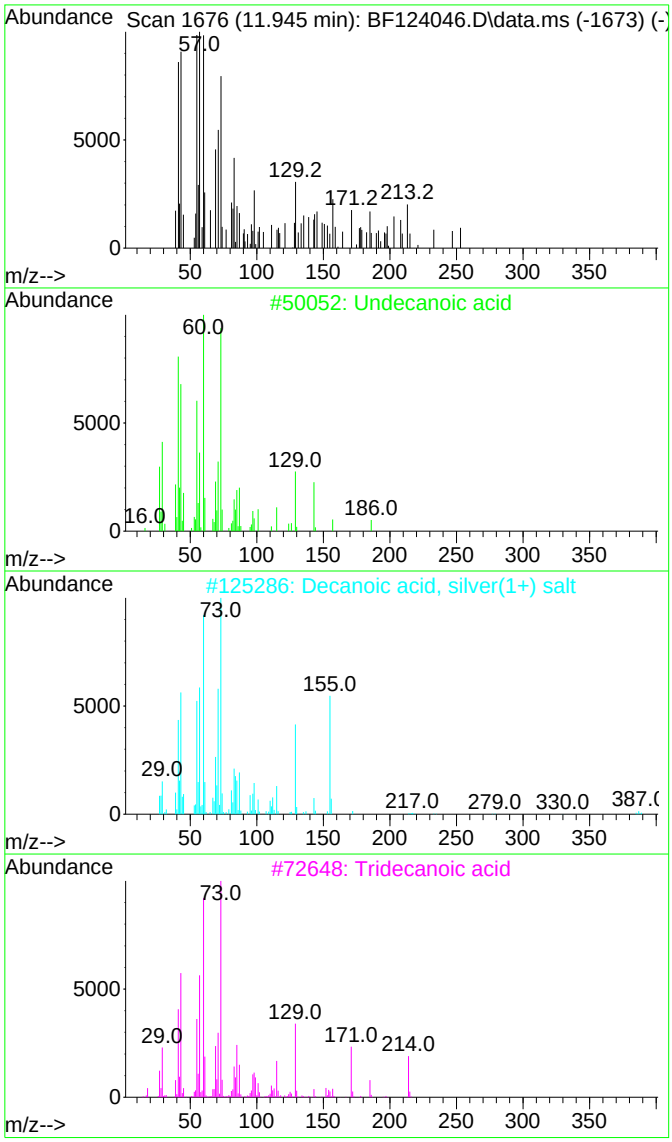
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

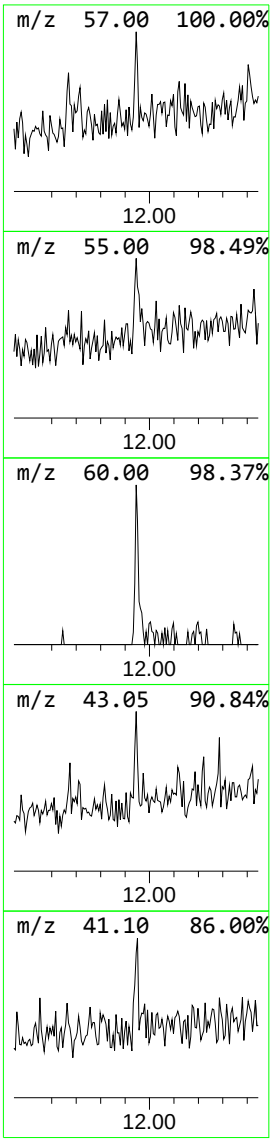
****

Peak Number 7 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.72 ng	50332	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	50
2	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	38
3	Tridecanoic acid	214	C13H26O2	000638-53-9	38
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	38
5	8-Chlorocapric acid	178	C8H15ClO2	001795-62-6	35





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Acq On : 24 May 2021 19:50
Operator : JU/CG
Sample : M2479-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUBBASE-6-1-D

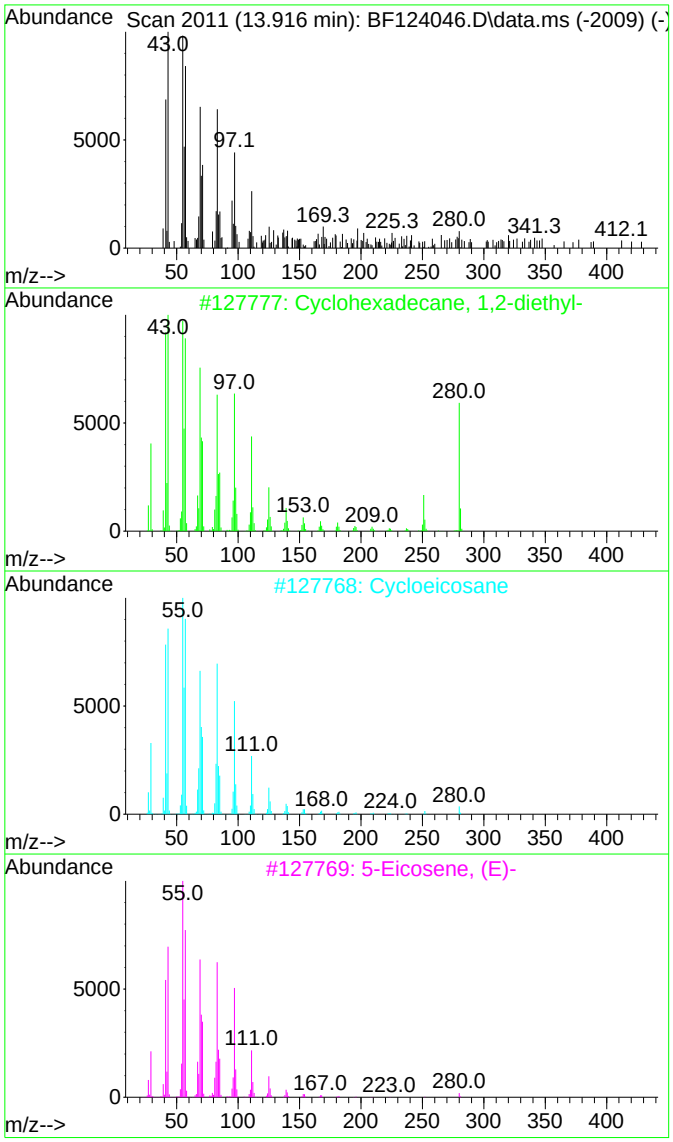
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

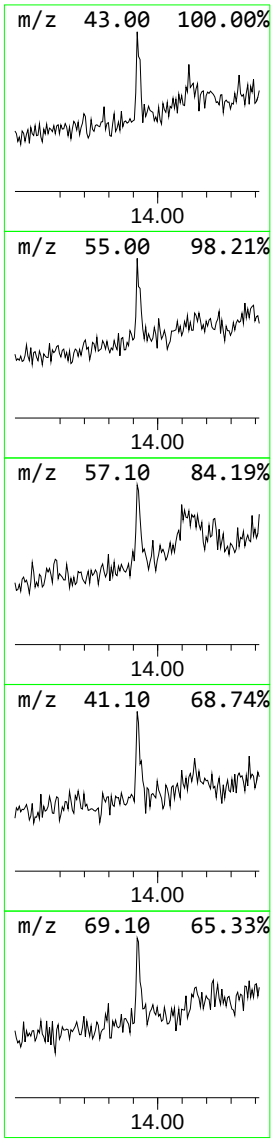
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclohexadecane, 1,2-diethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	11.80 ng	126233	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	94
2	Cycloeicosane	280	C20H40	000296-56-0	94
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4	E-7-Octadecene	252	C18H36	1000130-92-0	89
5	1-Eicosene	280	C20H40	003452-07-1	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124046.D
Acq On : 24 May 2021 19:50
Operator : JU/CG
Sample : M2479-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUBBASE-6-1-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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...	2.134	27.9	ng	433125	1	6.893	310333	20.0
Propane, 1,1-di...	2.240	2.5	ng	38197	1	6.893	310333	20.0
2-Pentanone, 4-...	5.104	11.4	ng	177530	1	6.893	310333	20.0
unknown9.369	9.369	2.6	ng	48768	3	9.934	371003	20.0
Hexadecane, 2,6...	10.851	4.0	ng	73160	4	11.422	370368	20.0
Hexadecane, 2,6...	11.316	3.0	ng	55421	4	11.422	370368	20.0
Undecanoic acid	11.945	2.7	ng	50332	4	11.422	370368	20.0
Cyclohexadecane...	13.916	11.8	ng	126233	5	14.069	213890	20.0