LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126069.D
Acq On : 8 Nov 2021 17:15
Operator : JU/CG
Sample : M4477-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T5-B2-NW

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126069.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	4	12	19	rVB	1830539	2265529	53.80%	7.729%
2	5.469	570	575	578	rBV	3849036	3766354	89.45%	12.849%
3	6.481	741	747	750	rBV	3917128	3850676	91.45%	13.137%
4	6.851	807	810	814	rBV	1249789	964180	22.90%	3.289%
5	7.416	900	906	909	rBV	2560272	2455998	58.33%	8.379%
6	8.034	1008	1011	1024	rBV	547206	588078	13.97%	2.006%
7	8.134	1024	1028	1031	rBV	1479620	1145160	27.20%	3.907%
8	9.210	1206	1211	1214	rBV	5291585	4210752	100.00%	14.365%
9	9.886	1322	1326	1337	rVB	1429243	1149570	27.30%	3.922%
10	10.669	1456	1459	1473	rVB	2156870	2060372	48.93%	7.029%
11	11.369	1574	1578	1582	rBV	1126967	958979	22.77%	3.272%
12	11.769	1643	1646	1650	rVB	80497	64779	1.54%	0.221%
13	12.475	1763	1766	1771	rVB	186508	156354	3.71%	0.533%
14	12.957	1844	1848	1851	rBV	4304295	3496809	83.04%	11.930%
15	13.498	1935	1940	1944	rBV	114801	115289	2.74%	0.393%
16	13.863	1998	2002	2014	rBV2	150992	288692	6.86%	0.985%
17	14.010	2022	2027	2030	rBV	968077	947515	22.50%	3.233%
18	14.868	2170	2173	2179	rVB	81046	83460	1.98%	0.285%
19	15.474	2271	2276	2280	rBV	596121	743354	17.65%	2.536%

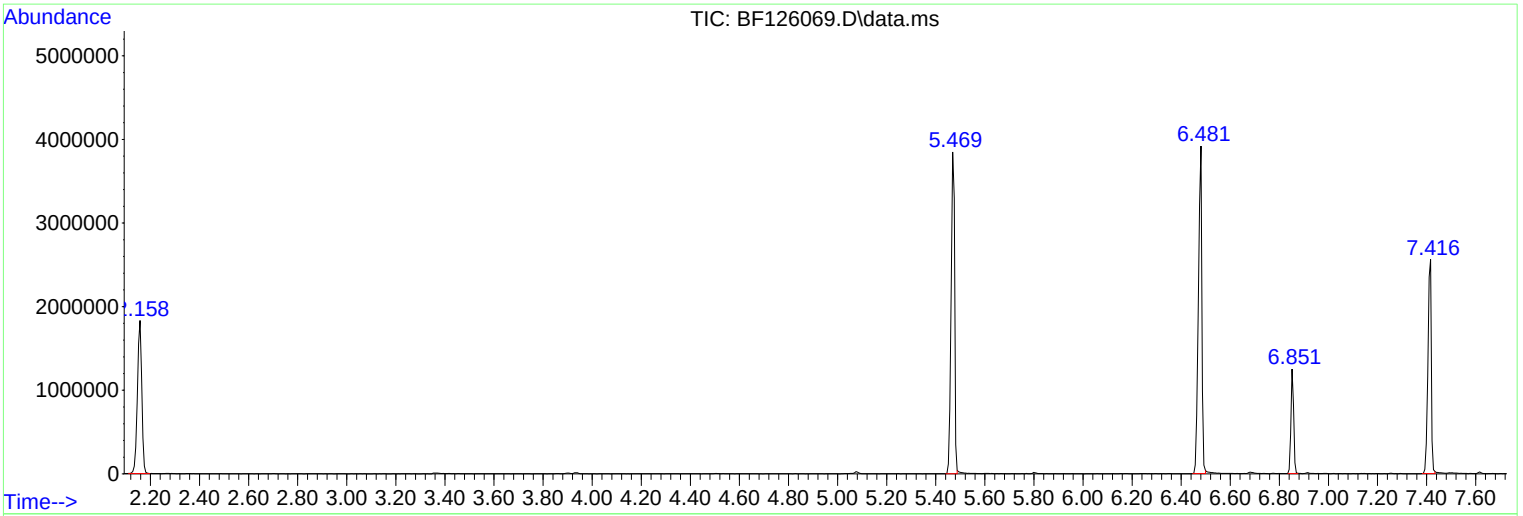
Sum of corrected areas: 29311900

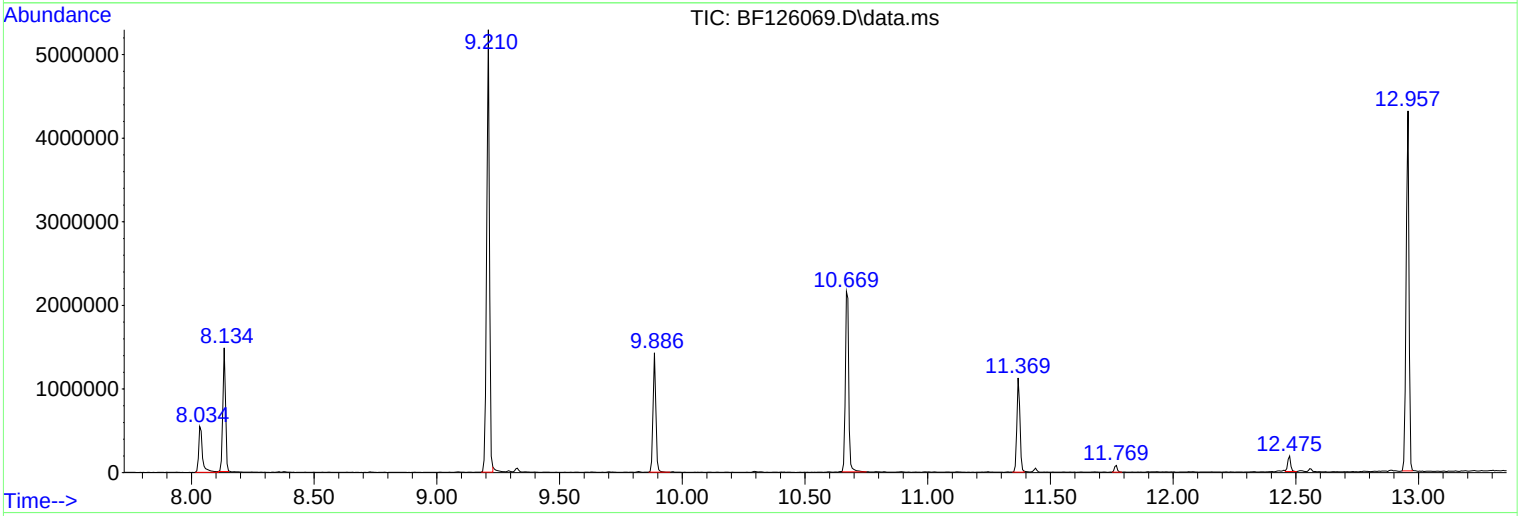
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126069.D
Acq On : 8 Nov 2021 17:15
Operator : JU/CG
Sample : M4477-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

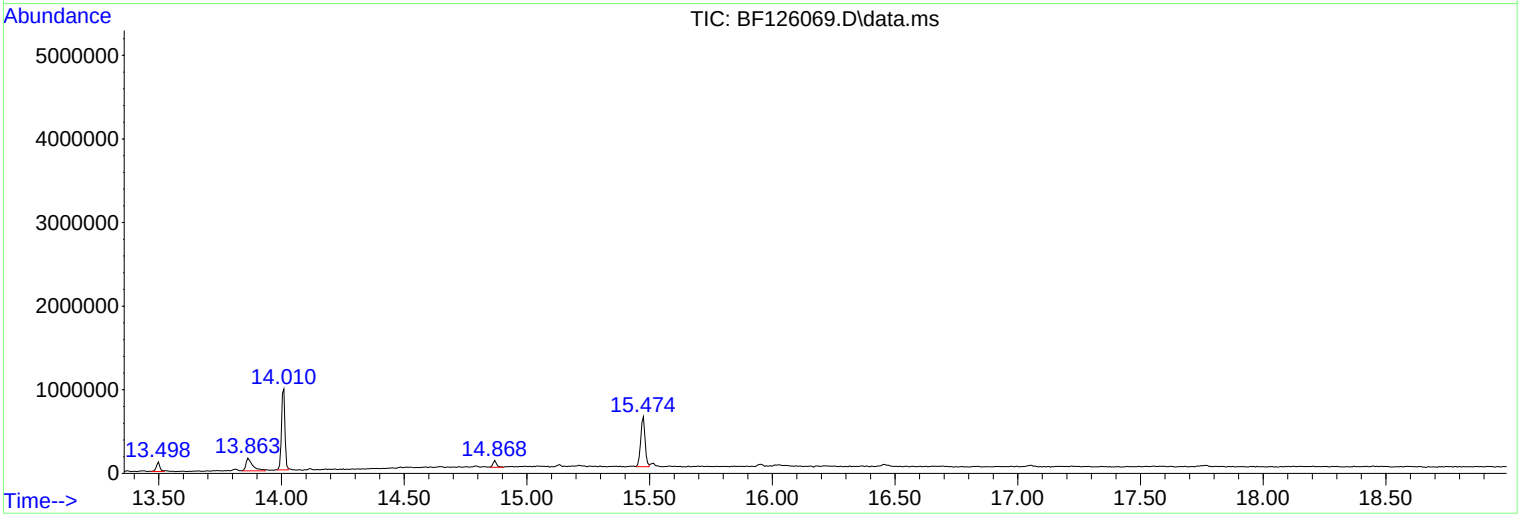
Instrument :
BNA_F
ClientSampleId :
T5-B2-NW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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\BF110821\
Data File : BF126069.D
Acq On : 8 Nov 2021 17:15
Operator : JU/CG
Sample : M4477-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T5-B2-NW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

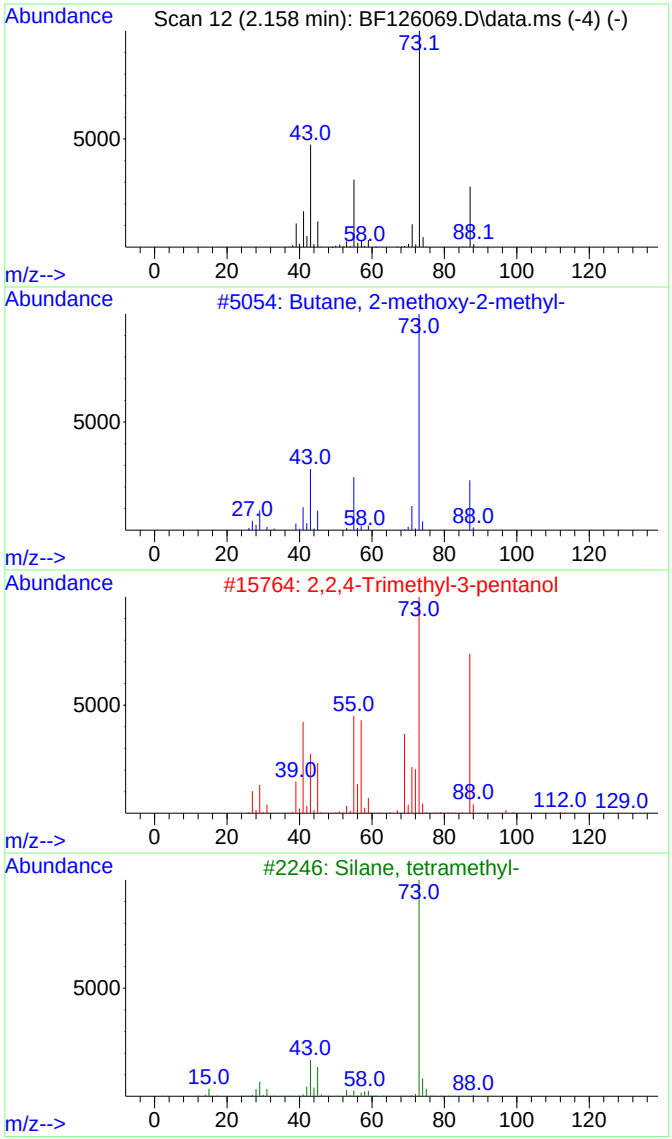
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

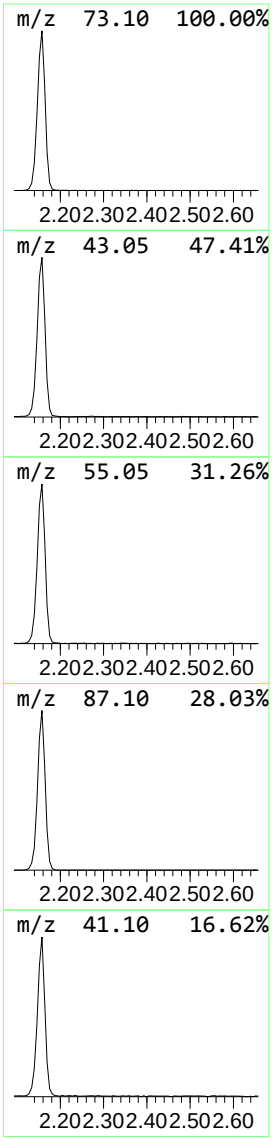
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.158	46.99 ng	2265530	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
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_F\Data\BF110821\
Data File : BF126069.D
Acq On : 8 Nov 2021 17:15
Operator : JU/CG
Sample : M4477-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T5-B2-NW

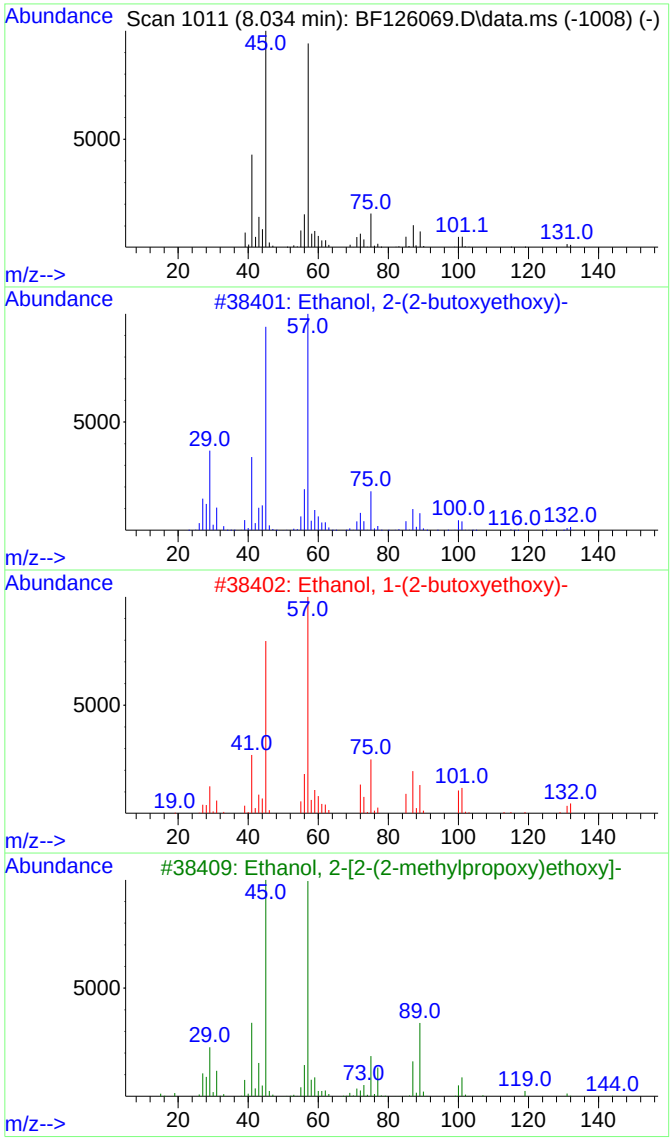
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

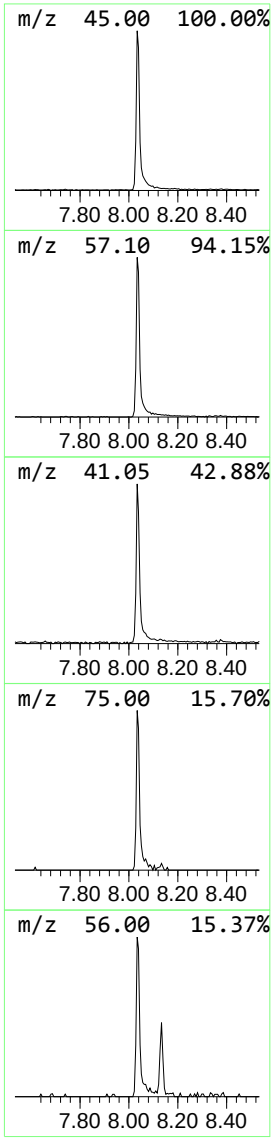
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.034	10.27 ng	588078	Naphthalene-d8	8.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5	Propanoic acid, 3-methoxy-2-meth...	132	C6H12O3	003852-11-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126069.D
Acq On : 8 Nov 2021 17:15
Operator : JU/CG
Sample : M4477-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T5-B2-NW

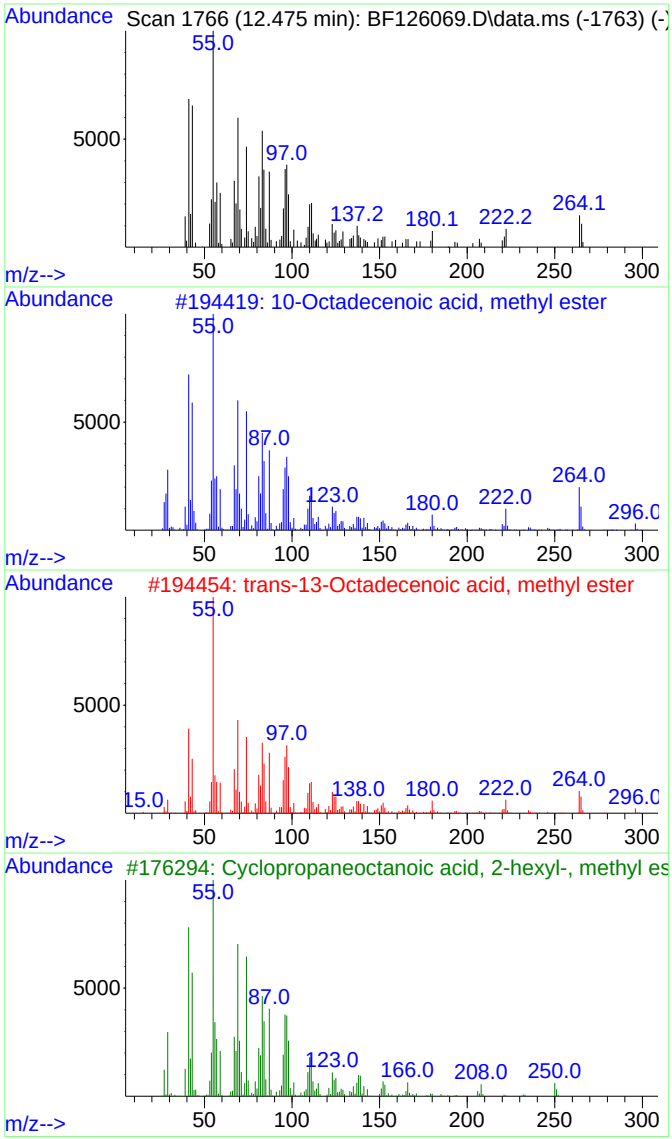
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

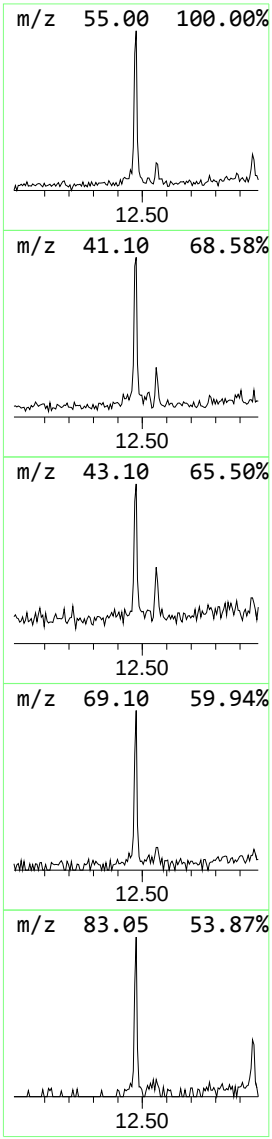
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 10-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.475	3.26 ng	156354	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	90
3	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	87
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	86
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126069.D
Acq On : 8 Nov 2021 17:15
Operator : JU/CG
Sample : M4477-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T5-B2-NW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

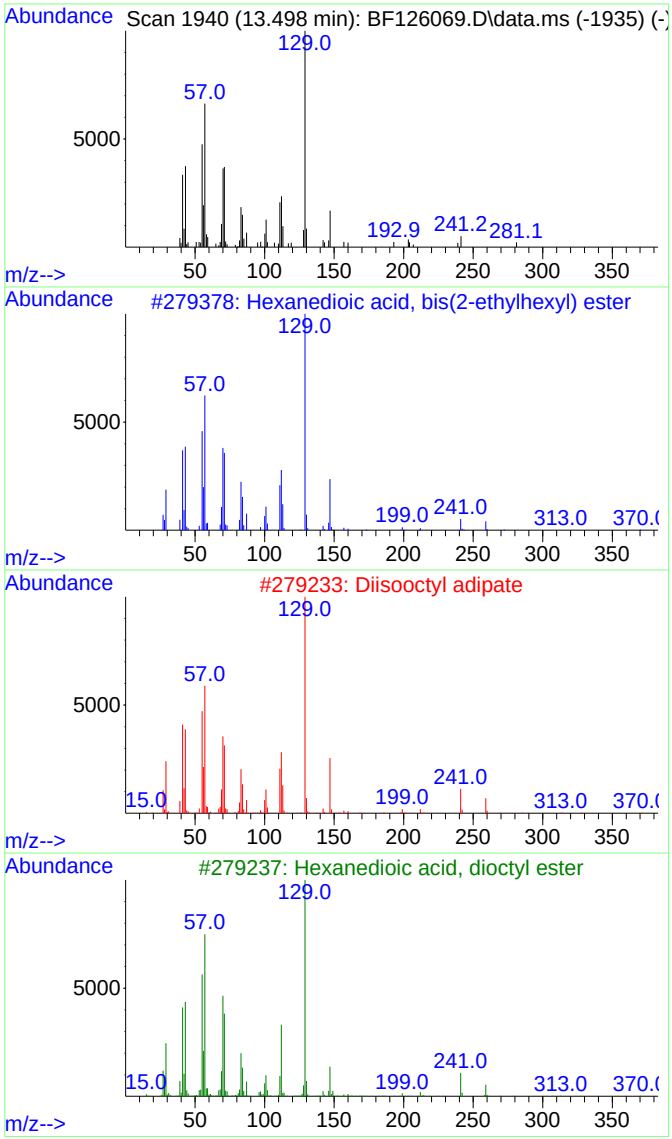
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

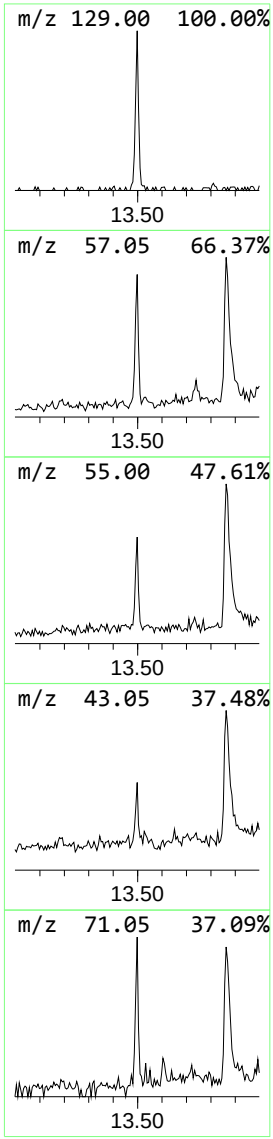
****

Peak Number 4 Hexanedioic acid, bis(2-eth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	2.43 ng	115289	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	95
2	Diisooctyl adipate	370	C22H42O4	001330-86-5	91
3	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	83
4	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	58
5	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126069.D
Acq On : 8 Nov 2021 17:15
Operator : JU/CG
Sample : M4477-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T5-B2-NW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

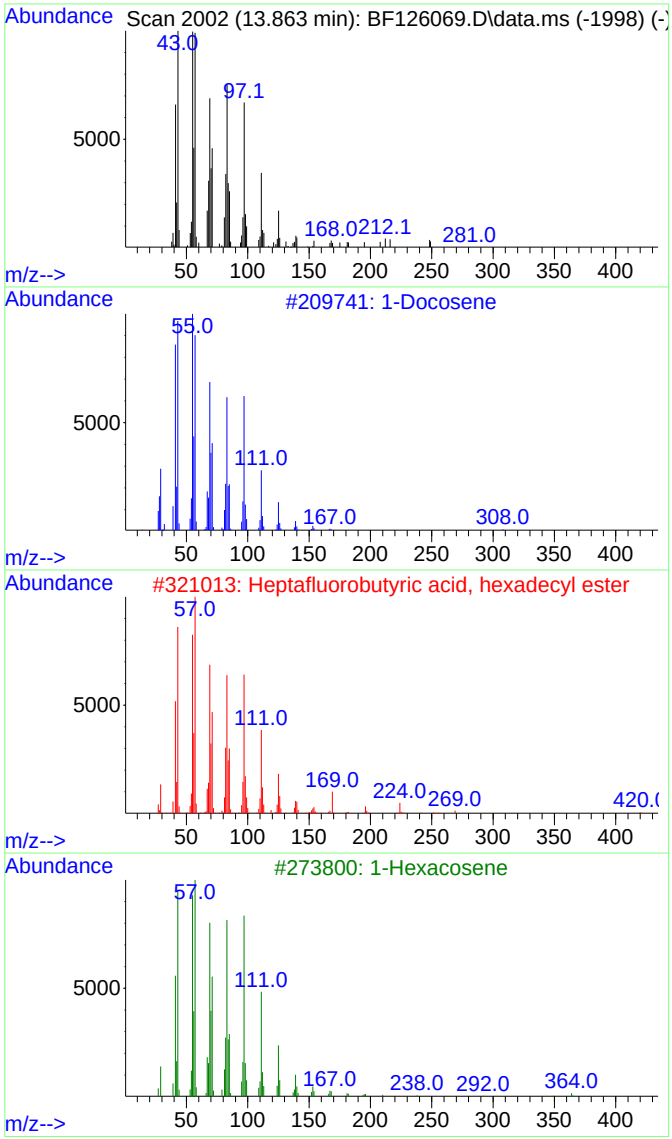
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

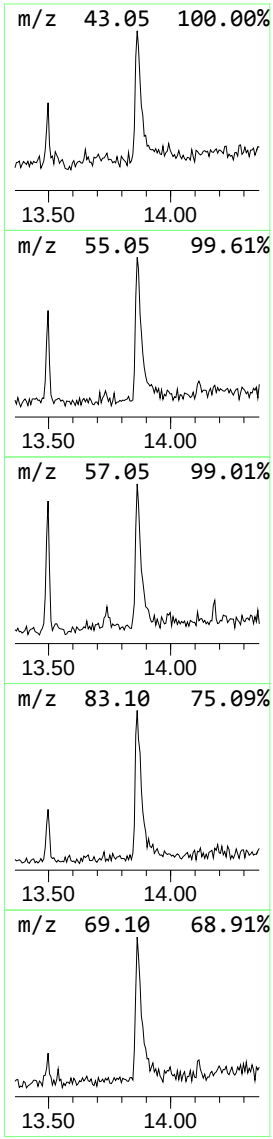
****

Peak Number 5 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	6.09 ng	288692	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3	1-Hexacosene	364	C26H52	018835-33-1	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126069.D
Acq On : 8 Nov 2021 17:15
Operator : JU/CG
Sample : M4477-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T5-B2-NW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

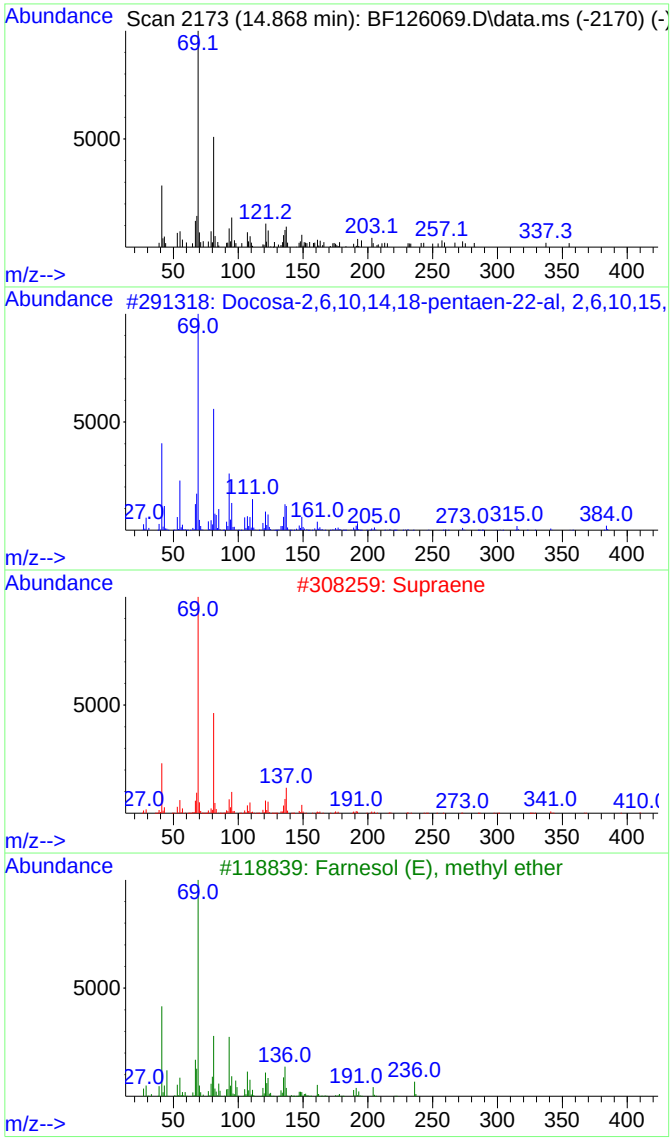
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

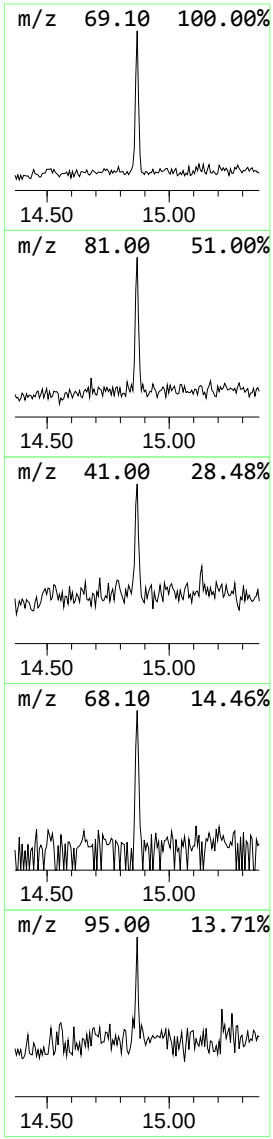
****

Peak Number 6 Docosa-2,6,10,14,18-pentaen... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	2.25 ng	83460	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
2	Supraene	410	C30H50	007683-64-9	72
3	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	64
4	3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	64
5	3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126069.D
Acq On : 8 Nov 2021 17:15
Operator : JU/CG
Sample : M4477-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T5-B2-NW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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
Butane, 2-metho...	2.158	47.0	ng	2265530	1	6.851	964180	20.0
Ethanol, 2-(2-b...	8.034	10.3	ng	588078	2	8.134	1145160	20.0
10-Octadecenoic...	12.475	3.3	ng	156354	4	11.369	958979	20.0
Hexanedioic aci...	13.498	2.4	ng	115289	5	14.010	947515	20.0
1-Docosene	13.863	6.1	ng	288692	5	14.010	947515	20.0
Docosa-2,6,10,1...	14.868	2.3	ng	83460	6	15.474	743354	20.0