LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140121.D
Acq On : 29 Oct 2024 19:29
Operator : RC/JU
Sample : P4598-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F11

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140121.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	11	20	27	rVB	1050286	1703215	56.38%	7.158%
2	4.510	404	411	418	rBV	416893	613153	20.30%	2.577%
3	5.116	506	514	523	rVB	308304	472749	15.65%	1.987%
4	5.510	574	581	586	rBV	1802513	2397684	79.36%	10.076%
5	5.587	590	594	602	rVB	60725	76720	2.54%	0.322%
6	6.504	744	750	756	rBV	1733823	2446257	80.97%	10.281%
7	6.887	810	815	820	rBV	655216	801229	26.52%	3.367%
8	7.445	904	910	915	rBV	1267935	1672860	55.37%	7.030%
9	7.698	948	953	958	rBV	45113	55746	1.85%	0.234%
10	8.169	1027	1033	1038	rBV	849059	1071267	35.46%	4.502%
11	8.381	1064	1069	1077	rVB2	25049	33515	1.11%	0.141%
12	9.239	1209	1215	1226	rBV	2218025	3021183	100.00%	12.697%
13	9.922	1326	1331	1345	rBV	961249	1235267	40.89%	5.191%
14	10.633	1447	1452	1459	rBV	468279	605651	20.05%	2.545%
15	10.710	1459	1465	1479	rVV	1371949	1809849	59.91%	7.606%
16	10.945	1496	1505	1513	rVB	65037	84162	2.79%	0.354%
17	11.410	1579	1584	1591	rBV	947856	1180273	39.07%	4.960%
18	11.933	1668	1673	1687	rBV	279098	457158	15.13%	1.921%
19	12.722	1802	1807	1821	rBV	37202	76302	2.53%	0.321%
20	12.998	1848	1854	1859	rBV	1823476	2320251	76.80%	9.751%
21	13.904	2002	2008	2028	rBV2	45217	151401	5.01%	0.636%
22	14.057	2028	2034	2045	rVB	513986	705957	23.37%	2.967%
23	14.839	2161	2167	2174	rBV4	22244	53089	1.76%	0.223%
24	15.557	2282	2289	2301	rBV	438581	750130	24.83%	3.152%

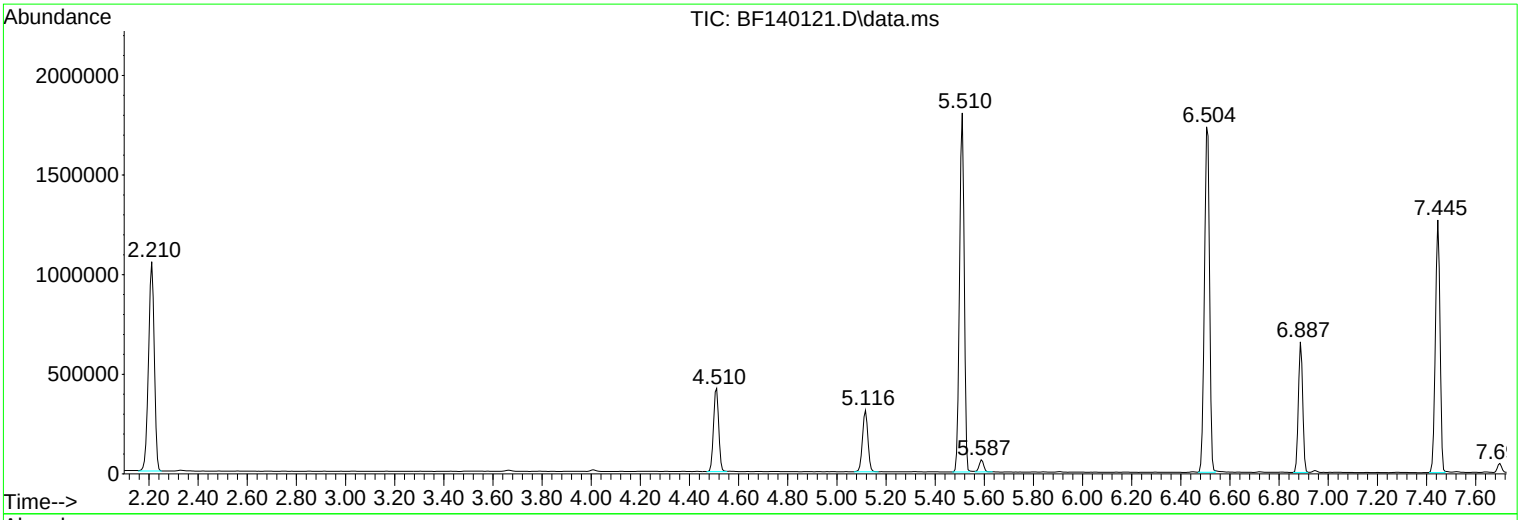
Sum of corrected areas: 23795068

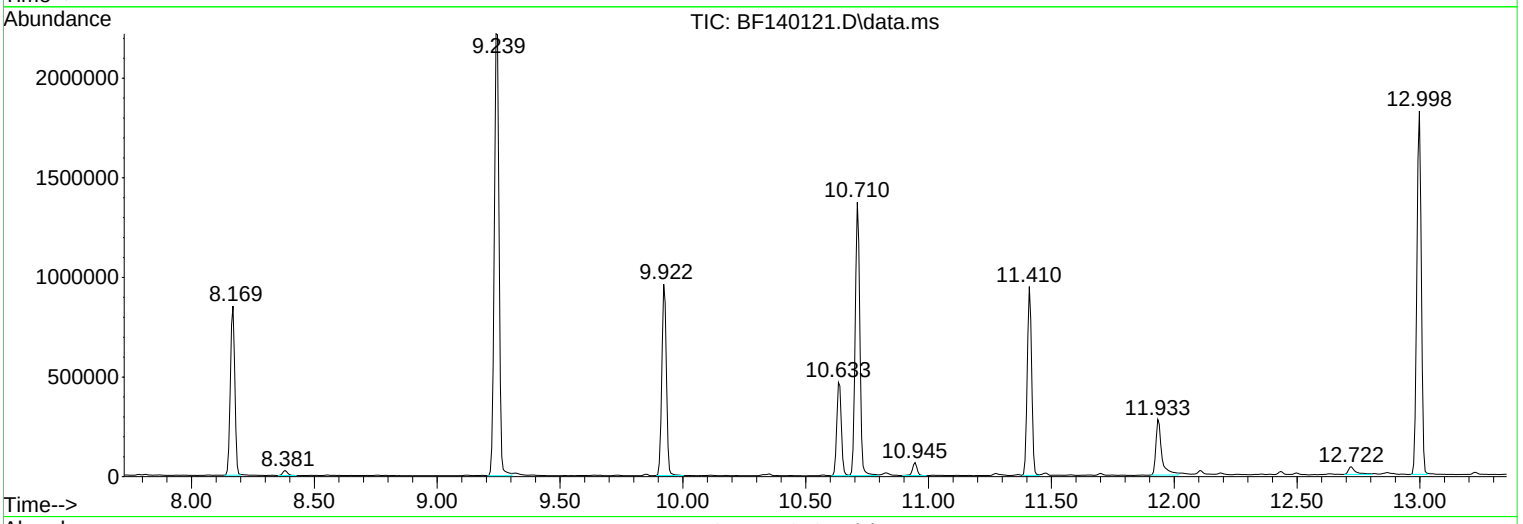
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140121.D
Acq On : 29 Oct 2024 19:29
Operator : RC/JU
Sample : P4598-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

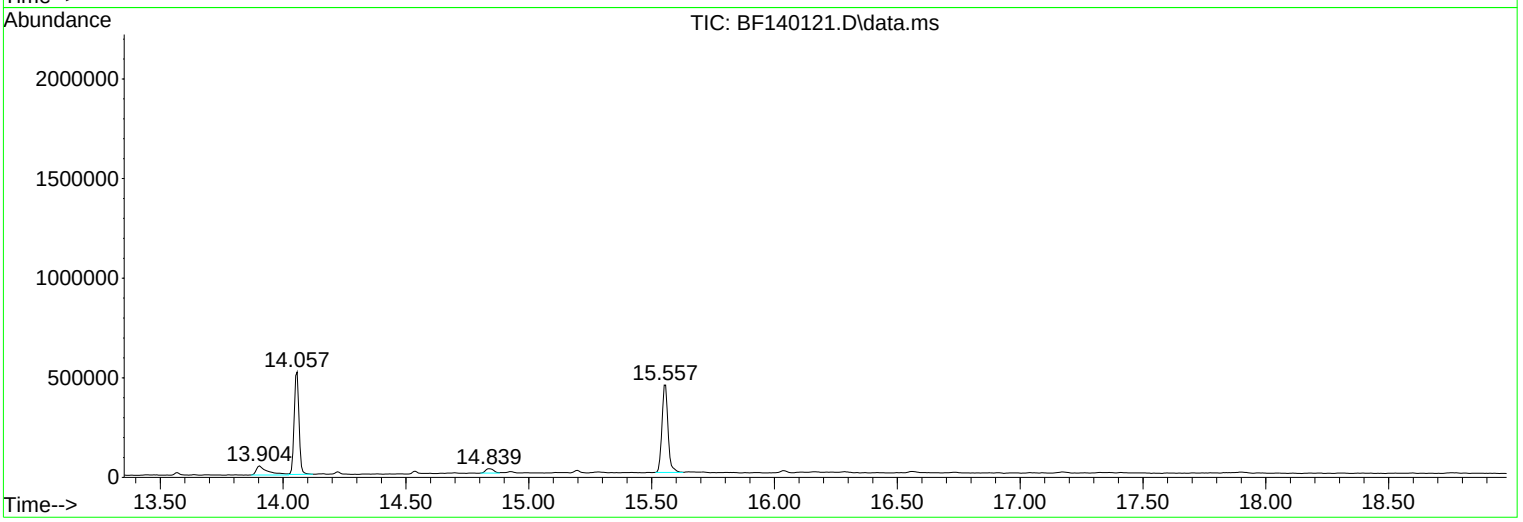
Instrument :
BNA_F
ClientSampleId :
BP-F11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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\BF102924\
Data File : BF140121.D
Acq On : 29 Oct 2024 19:29
Operator : RC/JU
Sample : P4598-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

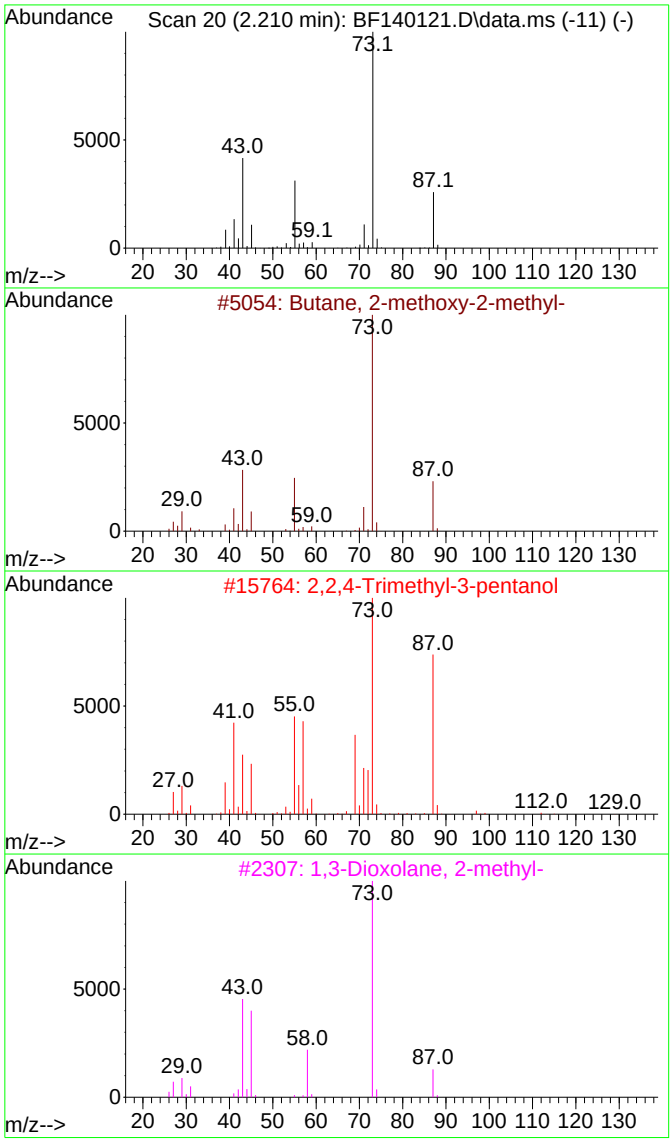
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

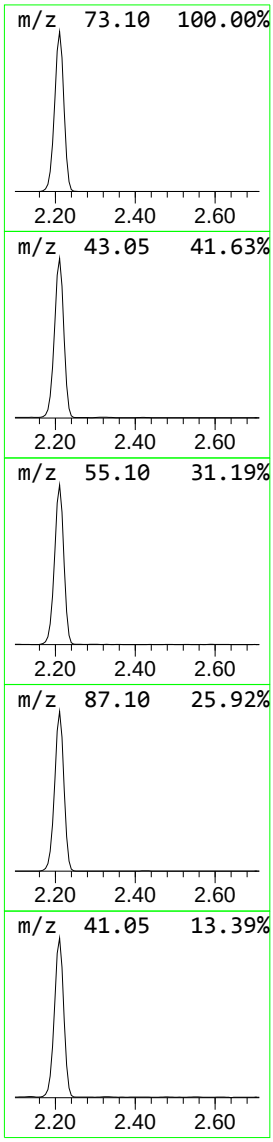
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	42.52 ng	1703220	1,4-Dichlorobenzene-d4	6.887

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140121.D
Acq On : 29 Oct 2024 19:29
Operator : RC/JU
Sample : P4598-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

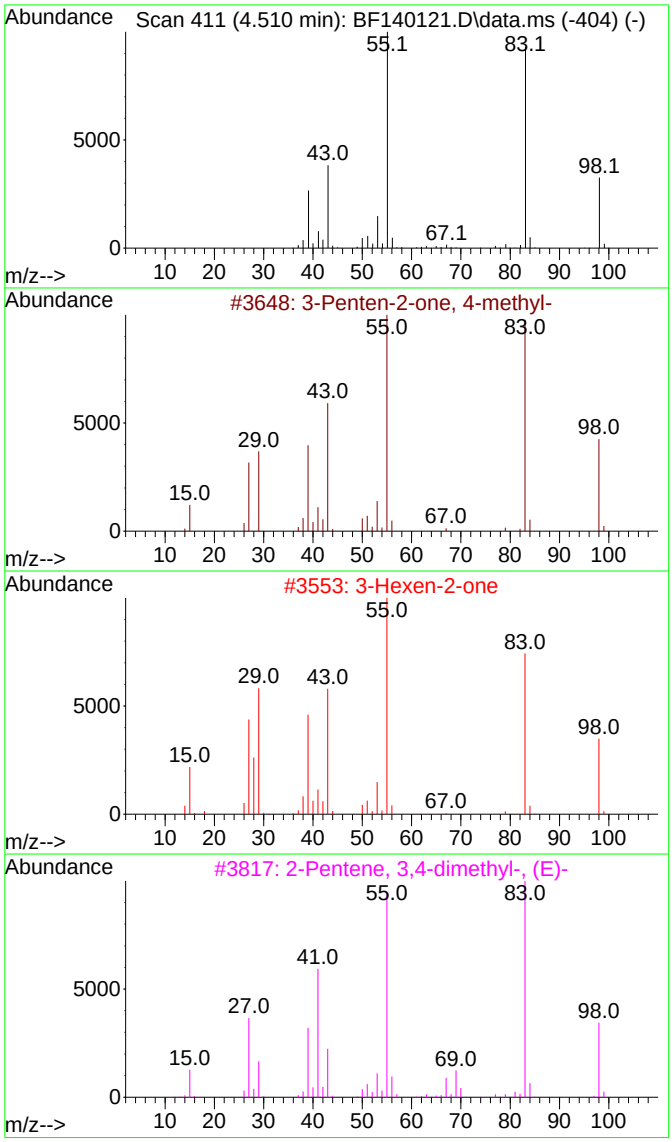
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

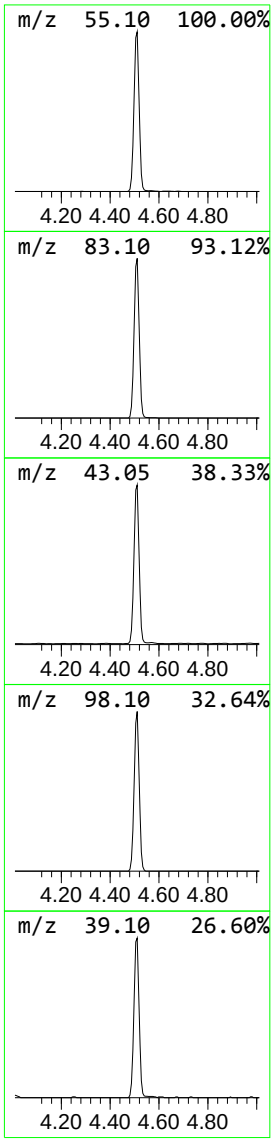
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	15.31 ng	613153	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140121.D
Acq On : 29 Oct 2024 19:29
Operator : RC/JU
Sample : P4598-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F11

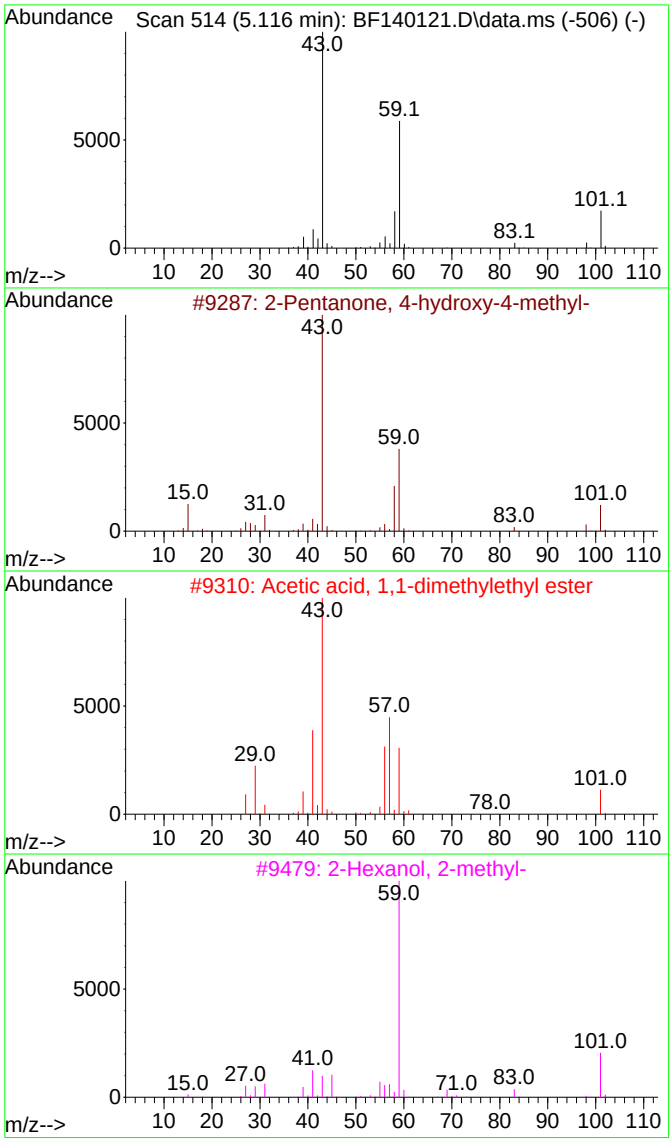
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

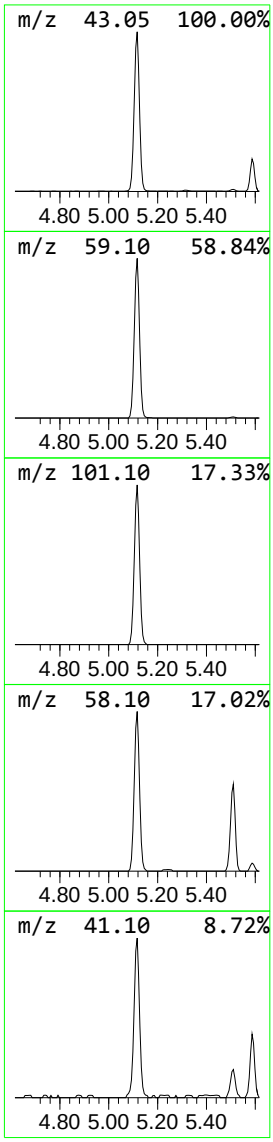
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	11.80 ng	472749	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140121.D
Acq On : 29 Oct 2024 19:29
Operator : RC/JU
Sample : P4598-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

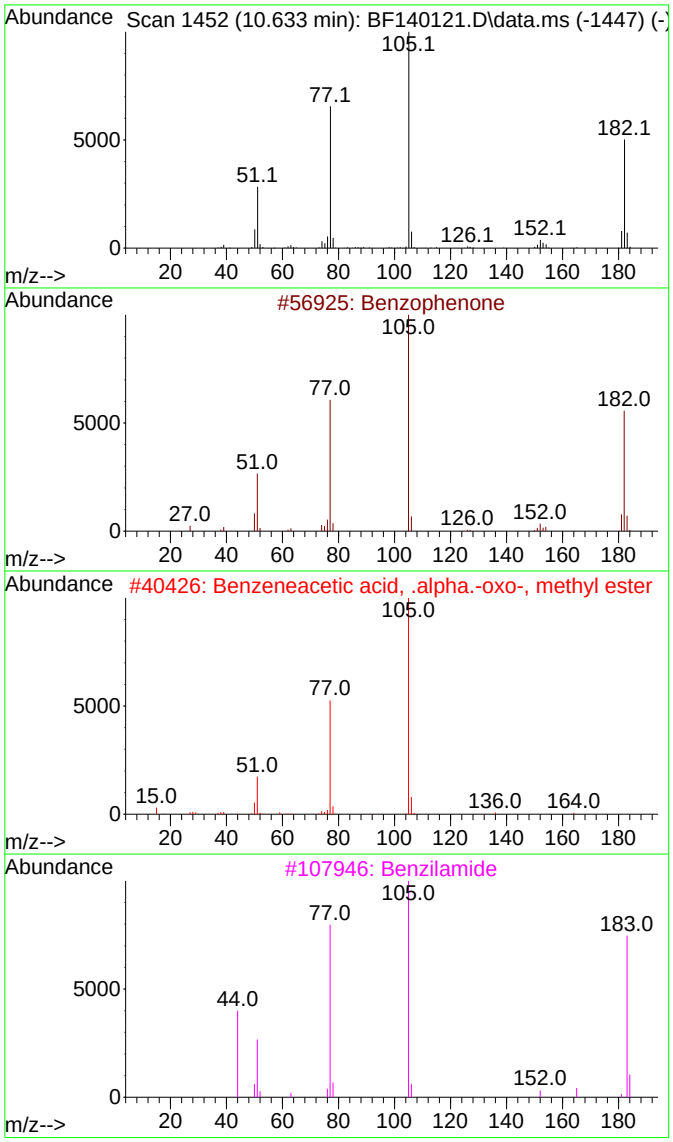
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

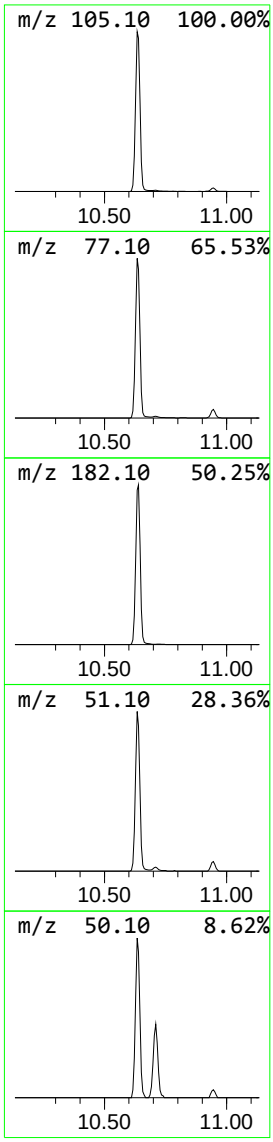
****

Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	9.81 ng	605651	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
3	Benzilamide	227	C14H13NO2	004746-87-6	47
4	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140121.D
Acq On : 29 Oct 2024 19:29
Operator : RC/JU
Sample : P4598-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

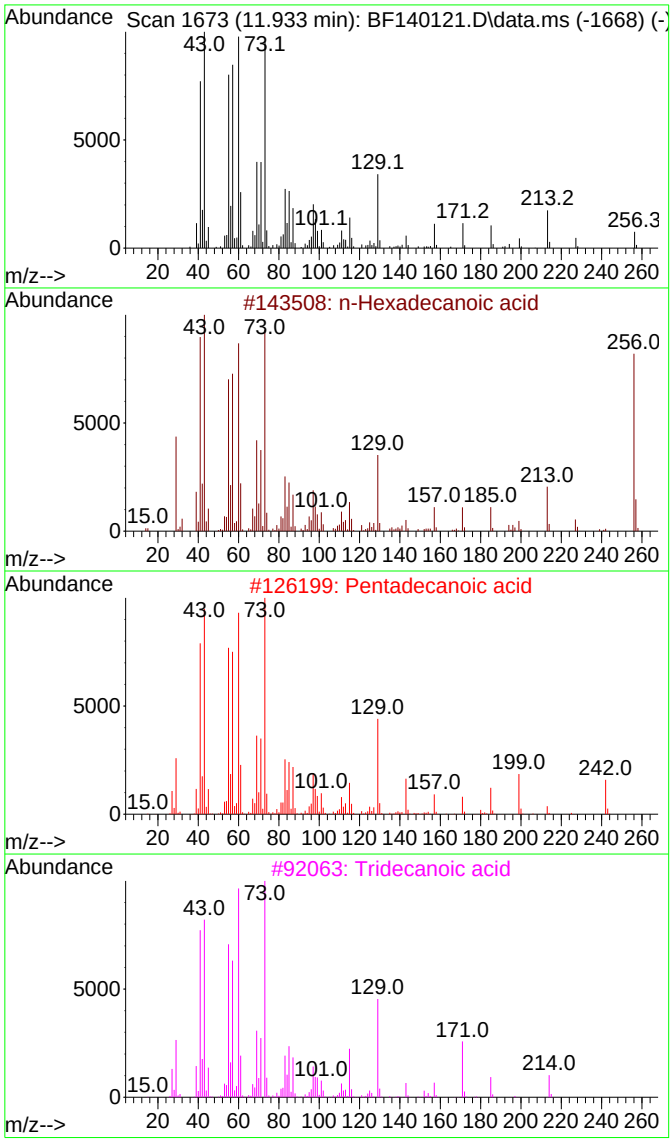
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

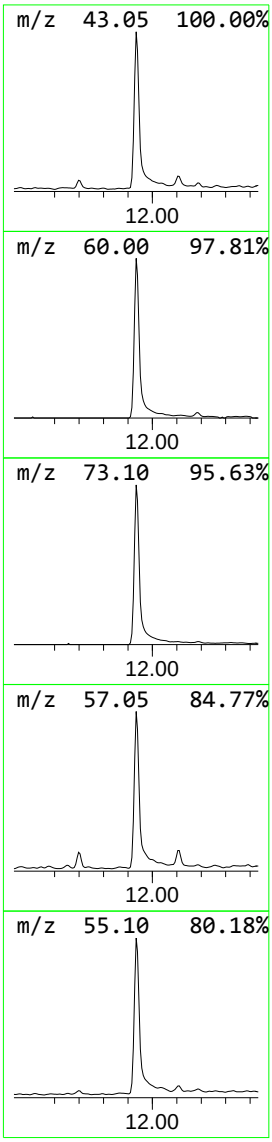
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	7.75 ng	457158	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140121.D
Acq On : 29 Oct 2024 19:29
Operator : RC/JU
Sample : P4598-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

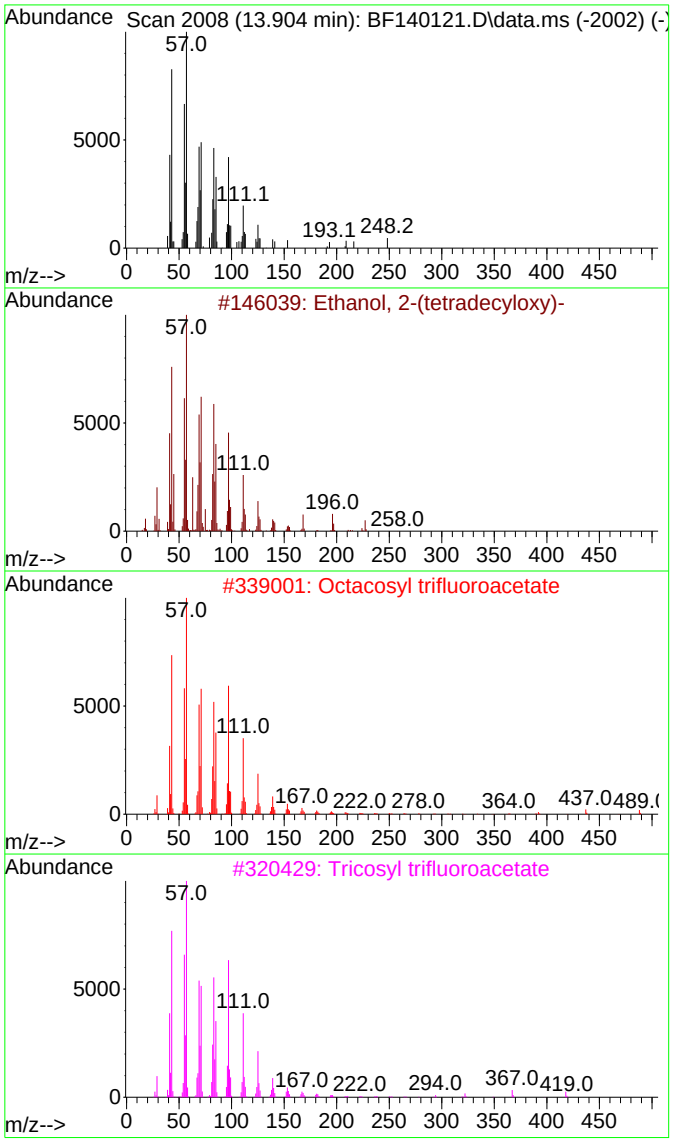
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

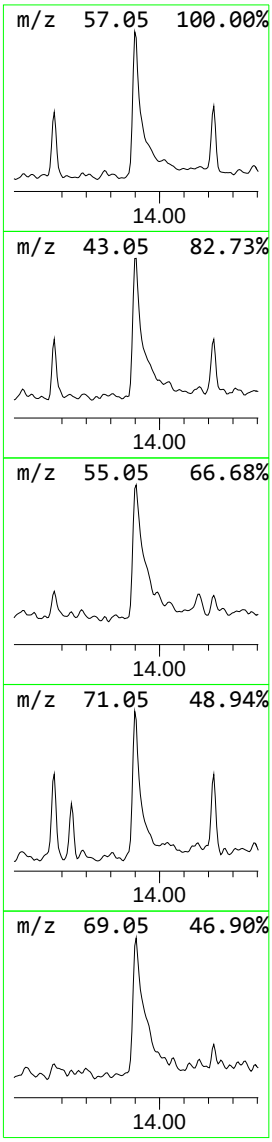
****

Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	4.29 ng	151401	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140121.D
Acq On : 29 Oct 2024 19:29
Operator : RC/JU
Sample : P4598-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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...	2.210	42.5	ng	1703220	1	6.887	801229	20.0
3-Penten-2-one,...	4.510	15.3	ng	613153	1	6.887	801229	20.0
2-Pentanone, 4-...	5.116	11.8	ng	472749	1	6.887	801229	20.0
Benzophenone	10.634	9.8	ng	605651	3	9.922	1235270	20.0
n-Hexadecanoic ...	11.933	7.8	ng	457158	4	11.410	1180270	20.0
Ethanol, 2-(tet...	13.904	4.3	ng	151401	5	14.057	705957	20.0