LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131119.D
Acq On : 10 Nov 2022 12:52
Operator : CG\JU
Sample : N5494-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131119.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	9	15	22	rVB	468703	591463	34.72%	5.062%
2	2.281	29	33	39	rVB	31192	40098	2.35%	0.343%
3	4.493	404	409	416	rBV	72525	85095	4.99%	0.728%
4	5.110	509	514	529	rVB	554555	646636	37.96%	5.534%
5	5.510	577	582	585	rBV	1918062	1703660	100.00%	14.581%
6	5.904	645	649	652	rBV	26487	22800	1.34%	0.195%
7	6.516	748	753	756	rBV	1518559	1391964	81.70%	11.913%
8	6.887	812	816	820	rBV	454577	350275	20.56%	2.998%
9	7.451	907	912	915	rBV	981426	865798	50.82%	7.410%
10	8.169	1030	1034	1038	rBV	507783	443004	26.00%	3.791%
11	9.251	1213	1218	1221	rBV	1635087	1532238	89.94%	13.113%
12	9.933	1329	1334	1337	rBV	578129	490210	28.77%	4.195%
13	10.722	1464	1468	1472	rBV	983965	898332	52.73%	7.688%
14	11.422	1584	1587	1591	rBV	537100	497923	29.23%	4.261%
15	13.016	1854	1858	1861	rBV	1549510	1335203	78.37%	11.427%
16	13.969	2013	2020	2031	rBV5	25883	81755	4.80%	0.700%
17	14.074	2034	2038	2041	rBV	380424	321691	18.88%	2.753%
18	14.168	2049	2054	2060	rBV	58756	58088	3.41%	0.497%
19	15.574	2287	2293	2299	rBV2	259952	328224	19.27%	2.809%

Sum of corrected areas: 11684457

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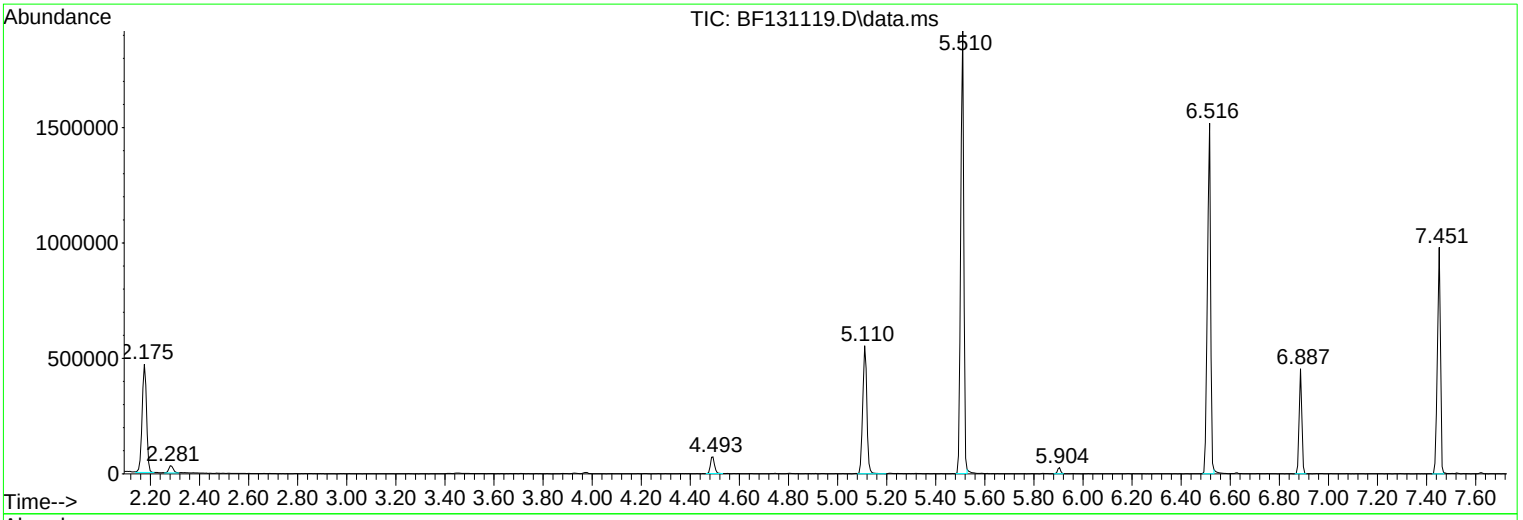
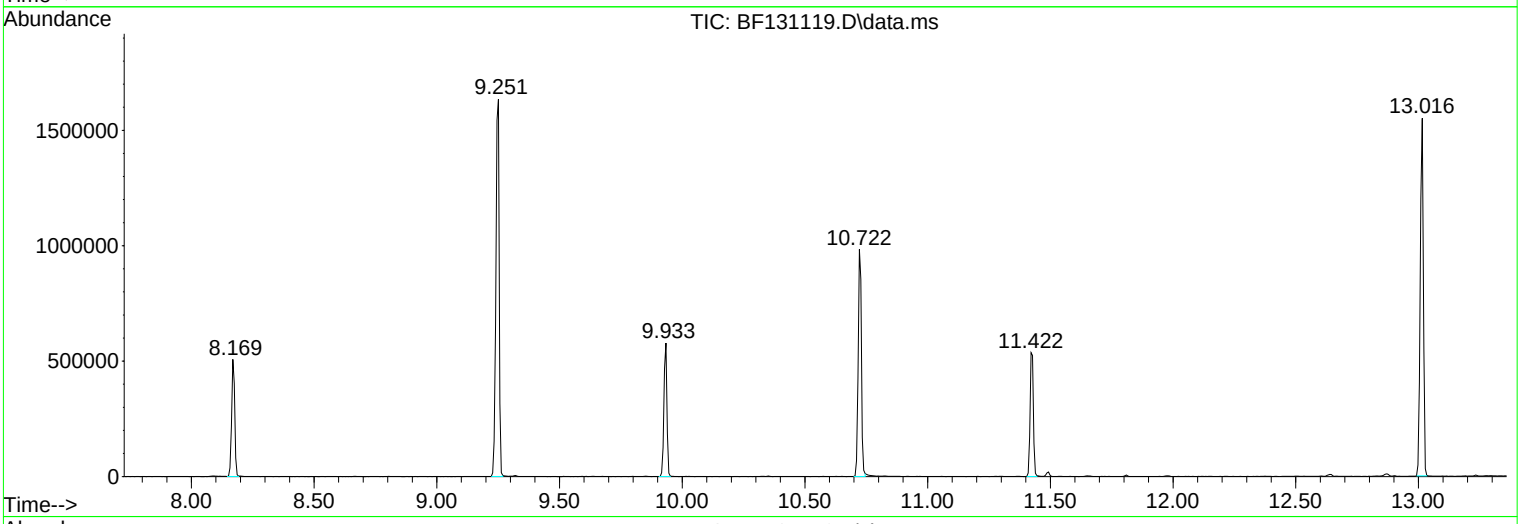
Misc :
ALS Vial : 6 Sample Multiplier: 1

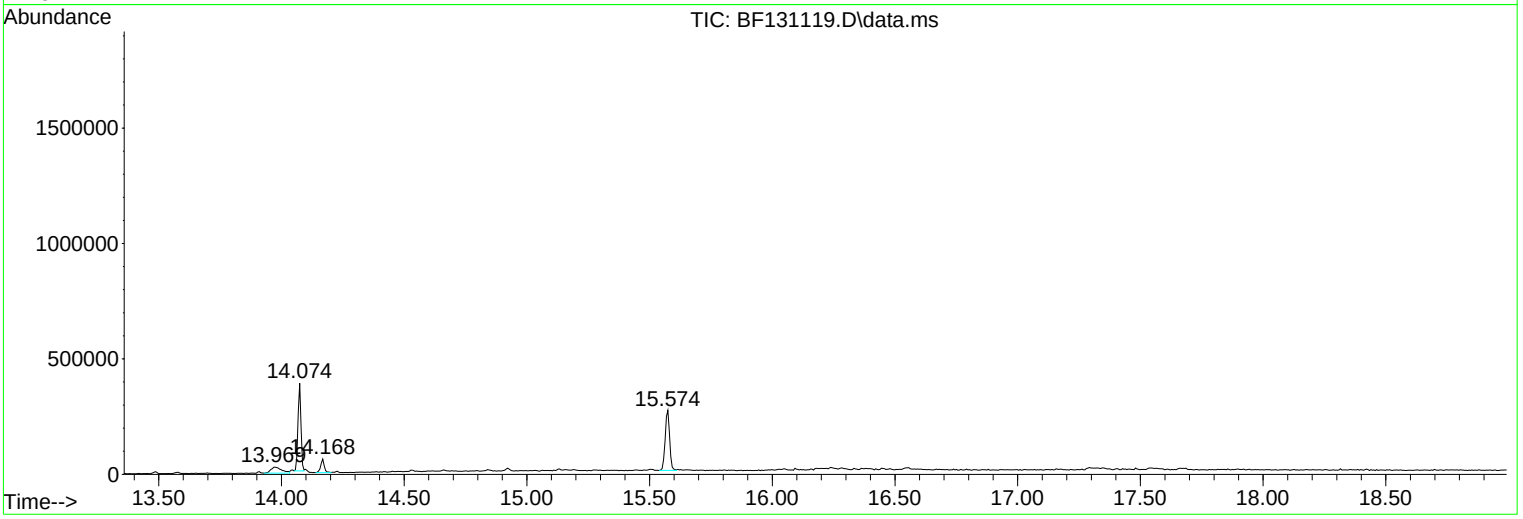
Instrument :
BNA_F
ClientSampleId :
SB-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BF131119.D
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

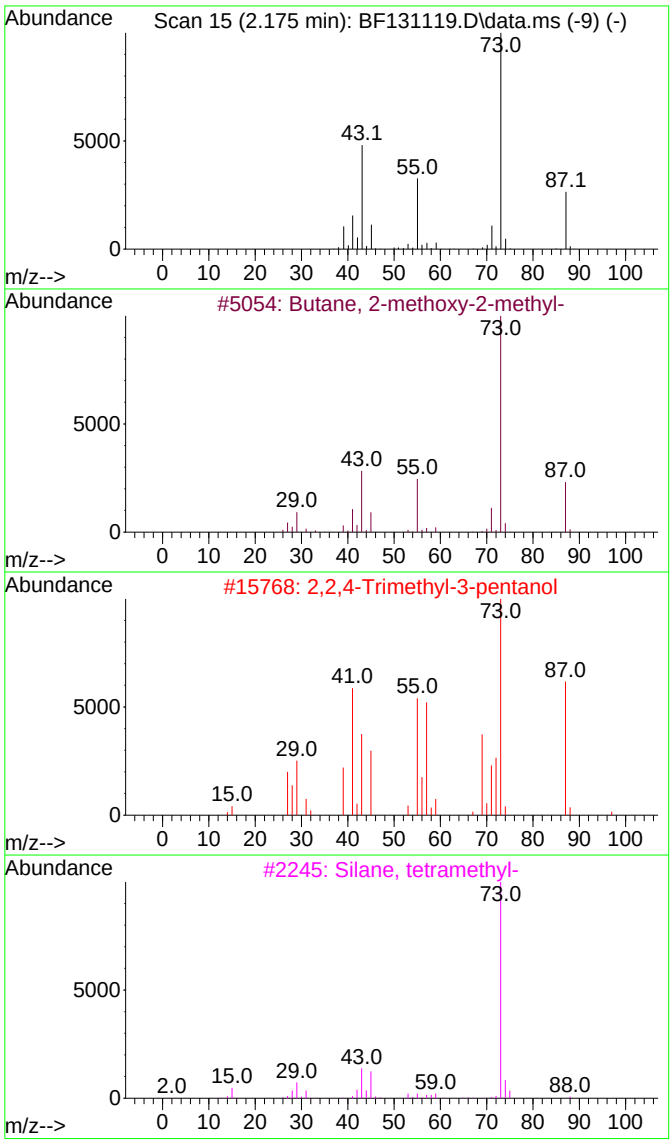
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

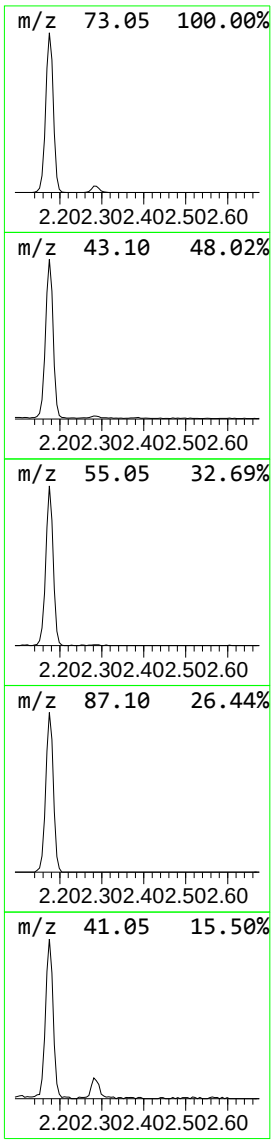
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	33.77 ng	591463	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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Data File : BF131119.D
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

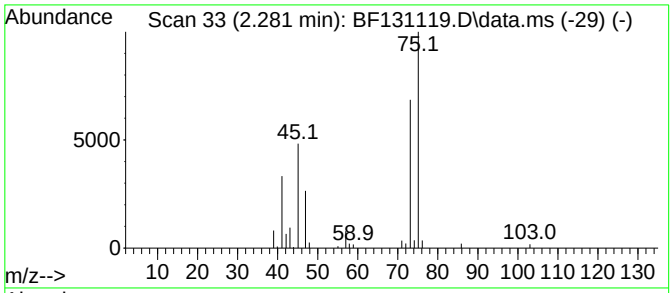
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

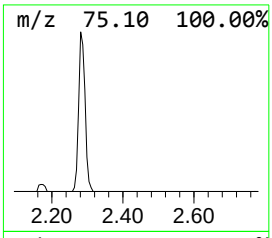
****

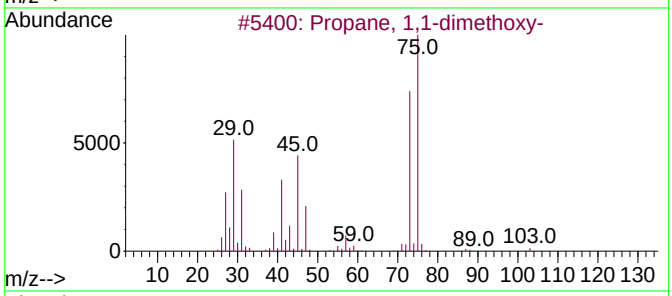
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

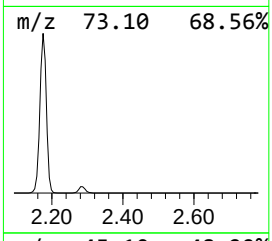
R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	2.29 ng	40098	1,4-Dichlorobenzene-d4	6.887

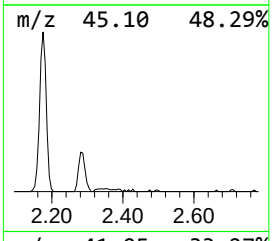
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36
3	Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	33
4	Glycine	75	C2H5NO2	000056-40-6	9
5	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	9

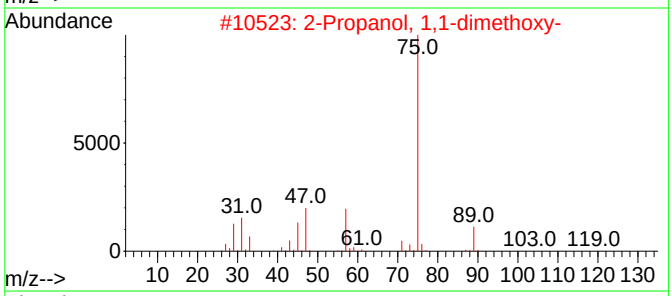


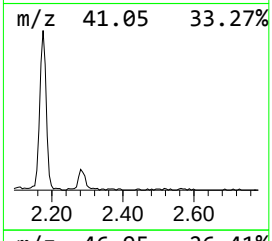


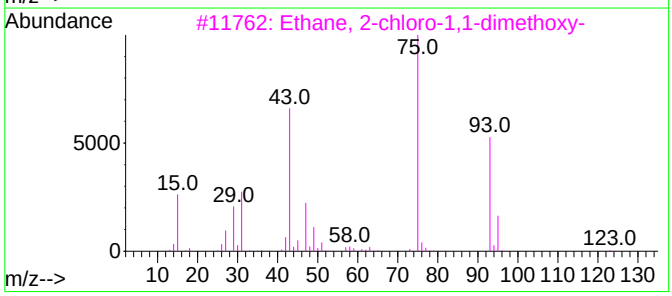


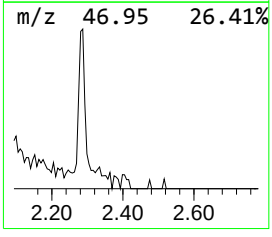












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Data File : BF131119.D
Acq On : 10 Nov 2022 12:52
Operator : CG\JU
Sample : N5494-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

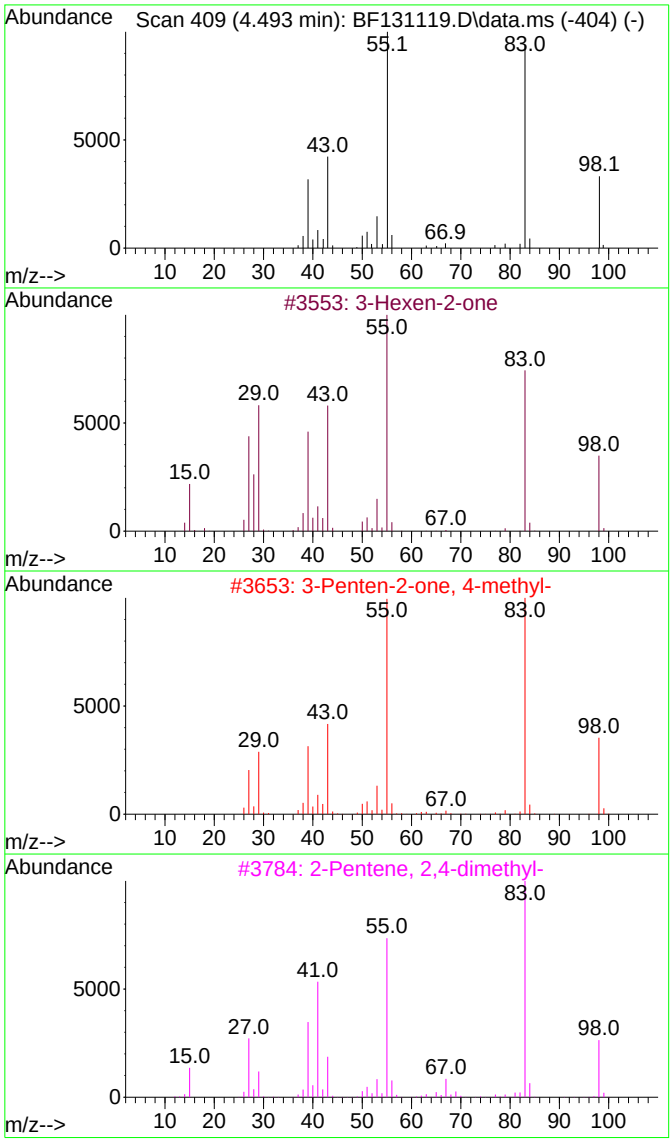
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

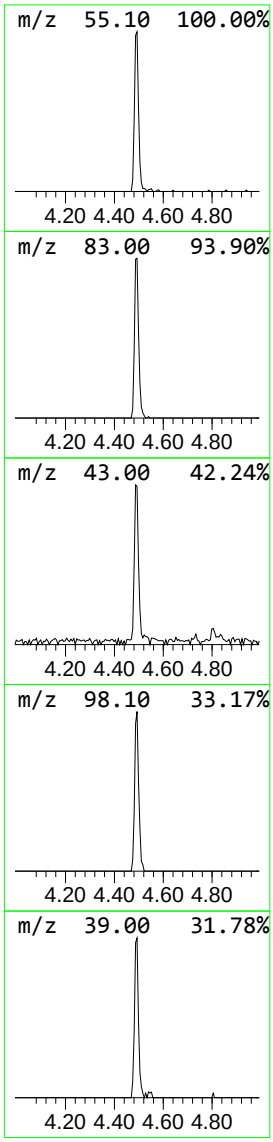
****

Peak Number 3 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.493	4.86 ng	85095	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4	Cyclopropane, 2-bromo-1,1,3-trim...	162	C6H11Br	036617-00-2	64
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	64





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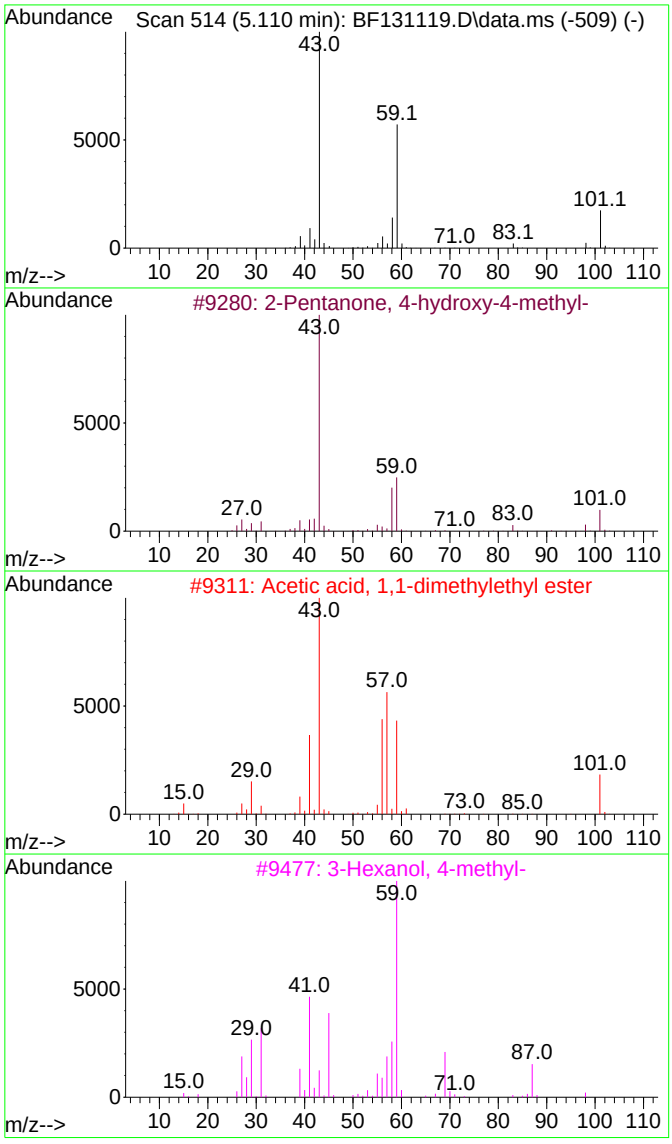
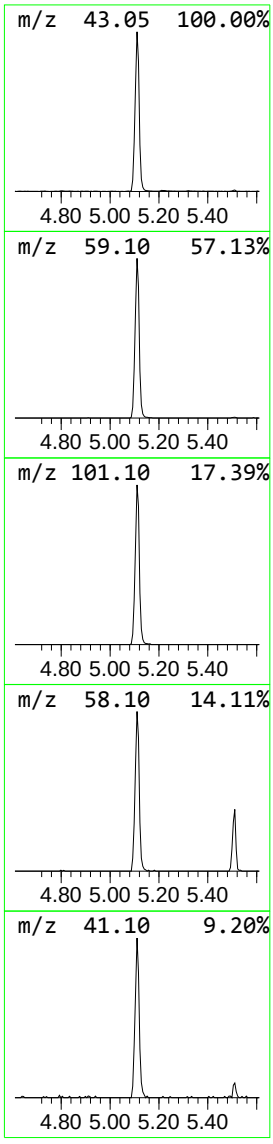
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	36.92 ng	646636	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	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131119.D
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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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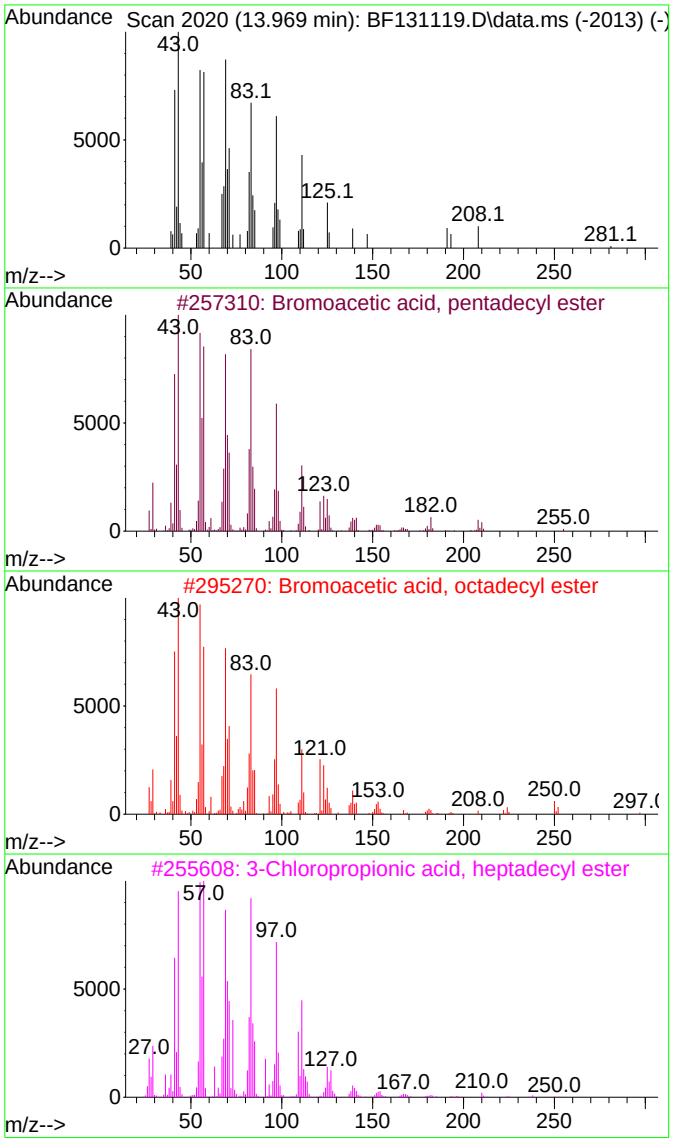
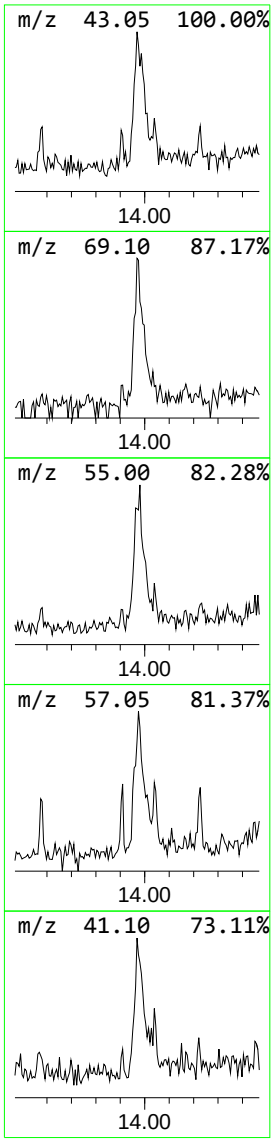
****
Peak Number 5 Bromoacetic acid, pentadecy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	5.08 ng	81755	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	87
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	81
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	81





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

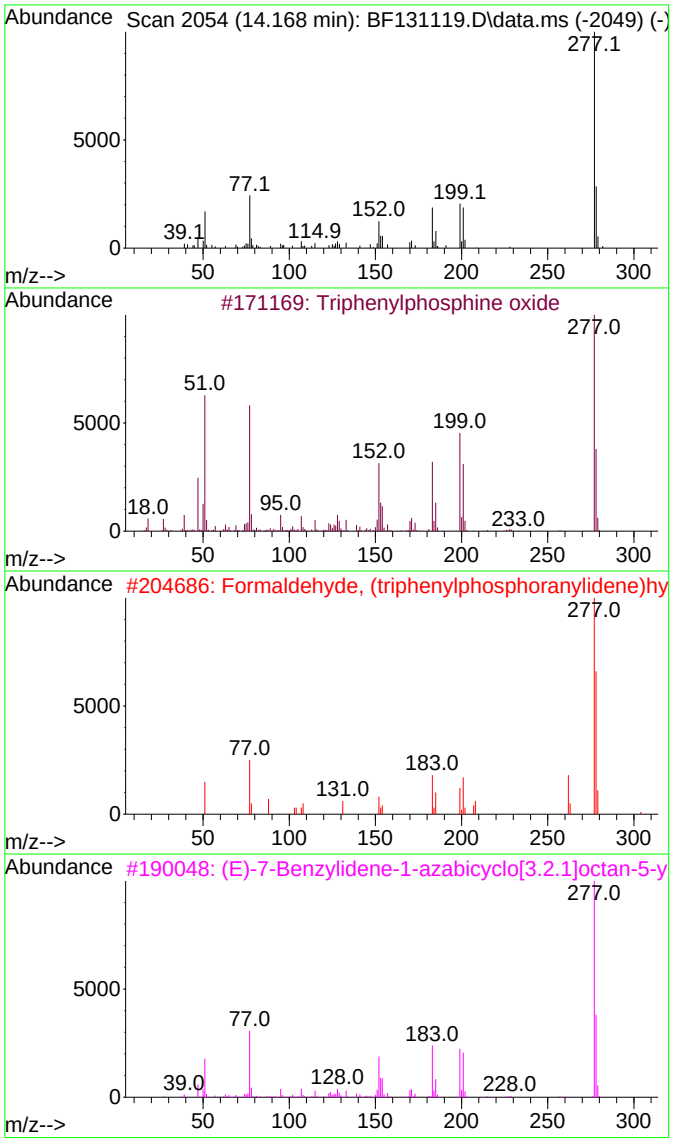
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

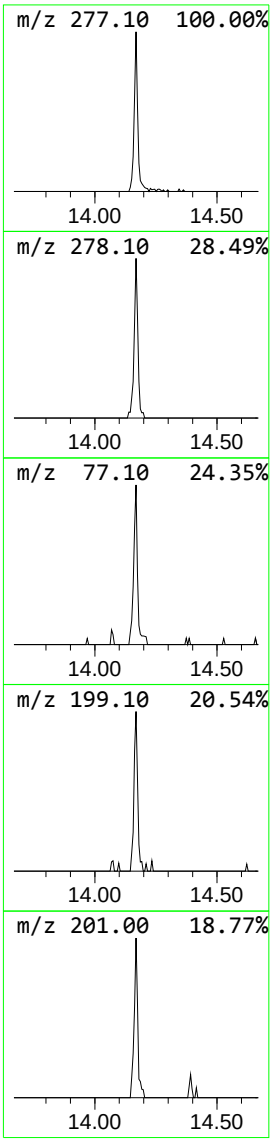
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	3.61 ng	58088	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	58
4	2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	50
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43





Tentatively Identified Compound (LSC) summary

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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...	2.175	33.8	ng	591463	1	6.887	350275	20.0
Propane, 1,1-di...	2.281	2.3	ng	40098	1	6.887	350275	20.0
3-Hexen-2-one	4.493	4.9	ng	85095	1	6.887	350275	20.0
2-Pentanone, 4-...	5.110	36.9	ng	646636	1	6.887	350275	20.0
Bromoacetic aci...	13.969	5.1	ng	81755	5	14.074	321691	20.0
Triphenylphosph...	14.169	3.6	ng	58088	5	14.074	321691	20.0