LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

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-BF112122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131396.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.275	24	32	37	rBV	1605894	2076903	67.06%	10.033%
2	3.369	210	218	223	rBV	50394	86816	2.80%	0.419%
3	4.498	405	410	419	rBV3	49186	82598	2.67%	0.399%
4	4.581	419	424	428	rBV	80185	90936	2.94%	0.439%
5	5.175	521	525	530	rVB	204233	212819	6.87%	1.028%
6	5.563	586	591	594	rBV	1612643	1428057	46.11%	6.898%
7	6.563	756	761	769	rBV	1025781	966737	31.22%	4.670%
8	6.710	777	786	790	rVB5	22744	35057	1.13%	0.169%
9	6.957	824	828	831	rBV	675842	586143	18.93%	2.831%
10	7.010	834	837	841	rBV	42714	33228	1.07%	0.161%
11	7.081	841	849	851	rBV3	17358	34114	1.10%	0.165%
12	7.134	853	858	863	rVB2	211449	255914	8.26%	1.236%
13	7.522	919	924	927	rVB	1939723	2092585	67.57%	10.108%
14	7.804	966	972	978	rVB2	85338	105540	3.41%	0.510%
15	7.975	998	1001	1007	rBV2	37938	43744	1.41%	0.211%
16	8.245	1042	1047	1049	rBV	882910	742020	23.96%	3.584%
17	8.263	1049	1050	1053	rVB	61888	42844	1.38%	0.207%
18	8.492	1085	1089	1094	rBV7	20608	36264	1.17%	0.175%
19	8.922	1158	1162	1164	rBV	66952	60959	1.97%	0.294%
20	9.057	1182	1185	1187	rBV	61444	50589	1.63%	0.244%
21	9.328	1225	1231	1234	rBV	3458813	3097015	100.00%	14.960%
22	9.492	1255	1259	1262	rVB	45234	38960	1.26%	0.188%
23	10.010	1341	1347	1350	rBV	1073100	847767	27.37%	4.095%
24	10.198	1372	1379	1384	rVB9	25717	34393	1.11%	0.166%
25	10.727	1463	1469	1472	rBV	197716	165936	5.36%	0.802%
26	10.804	1476	1482	1485	rBV	2264004	2045830	66.06%	9.883%
27	11.204	1547	1550	1555	rBV	33167	36892	1.19%	0.178%
28	11.504	1597	1601	1605	rBV	907105	796879	25.73%	3.849%
29	12.027	1686	1690	1702	rBV	454915	426759	13.78%	2.062%
30	12.280	1730	1733	1736	rBV	40538	35449	1.14%	0.171%
31	12.821	1821	1825	1832	rBV	362075	364426	11.77%	1.760%
32	13.104	1868	1873	1876	rBV	2790464	2535091	81.86%	12.246%
33	14.015	2023	2028	2039	rBV3	79359	179439	5.79%	0.867%
34	14.163	2050	2053	2057	rVB	552692	461287	14.89%	2.228%
35	14.263	2065	2070	2076	rVB	70736	77540	2.50%	0.375%
36	15.704	2309	2315	2319	rBV	373857	493786	15.94%	2.385%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

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-BF112122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

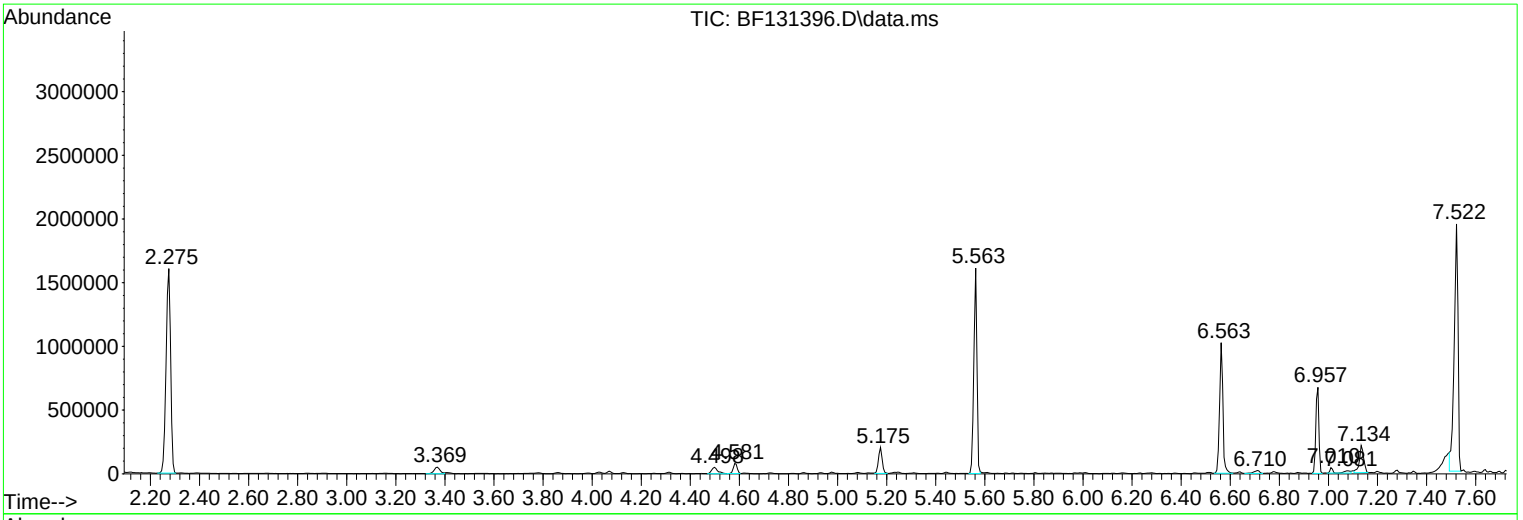
Sum of corrected areas: 20701316

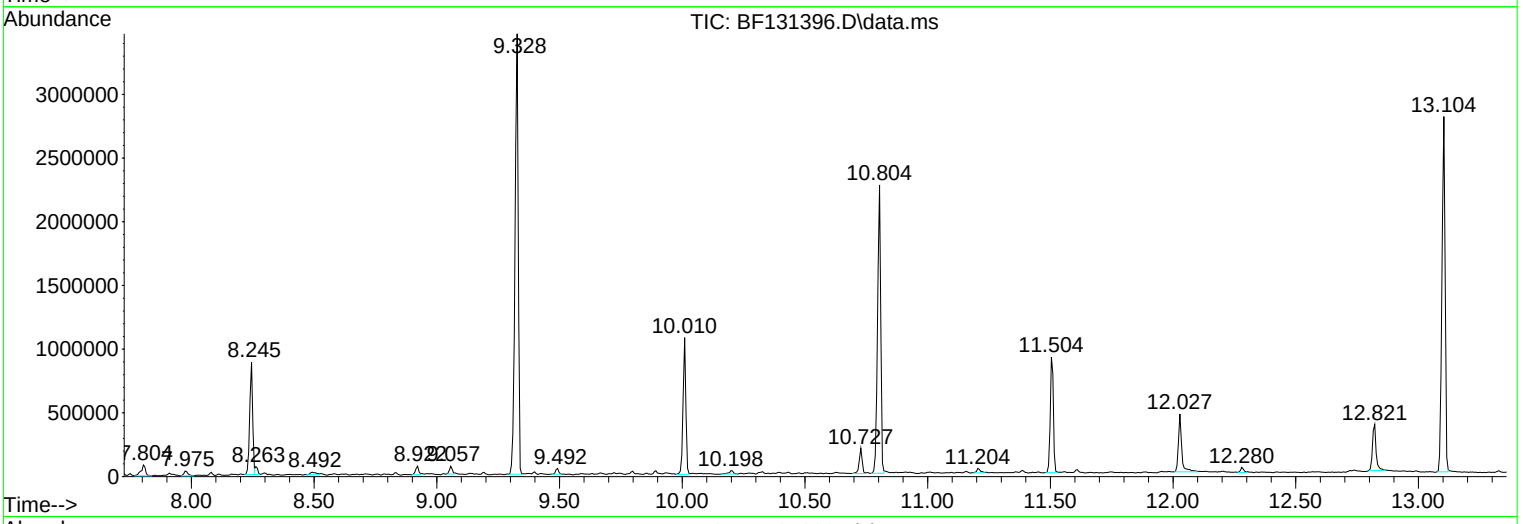
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

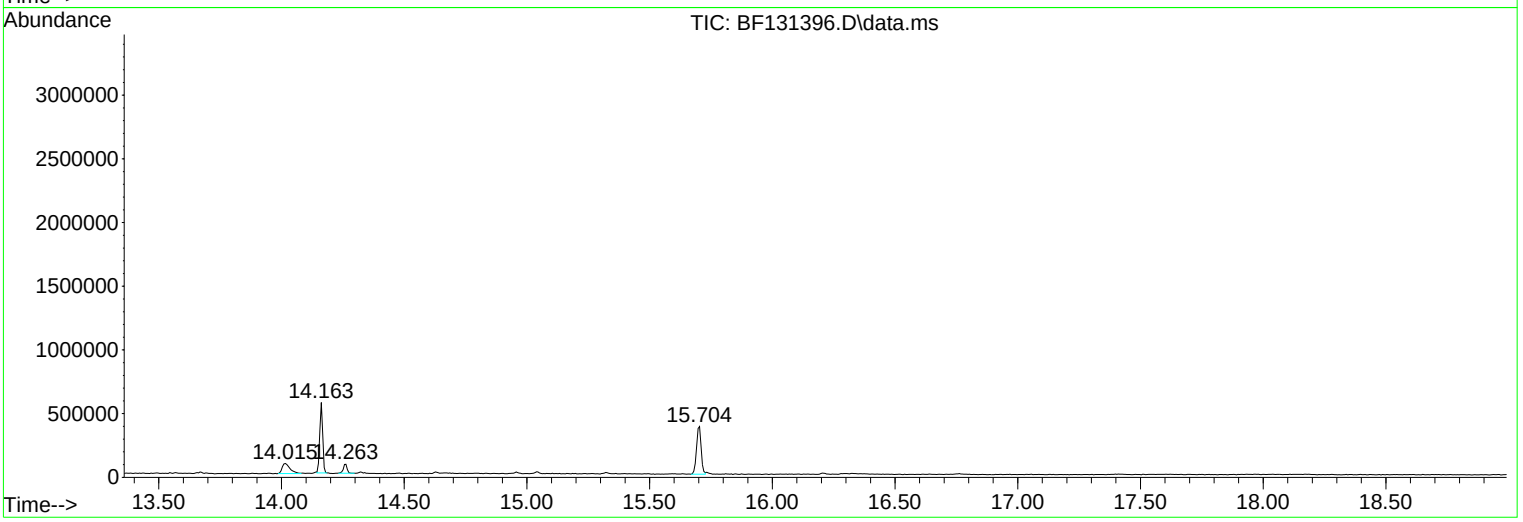
Instrument :
BNA_F
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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\BF112522\
Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

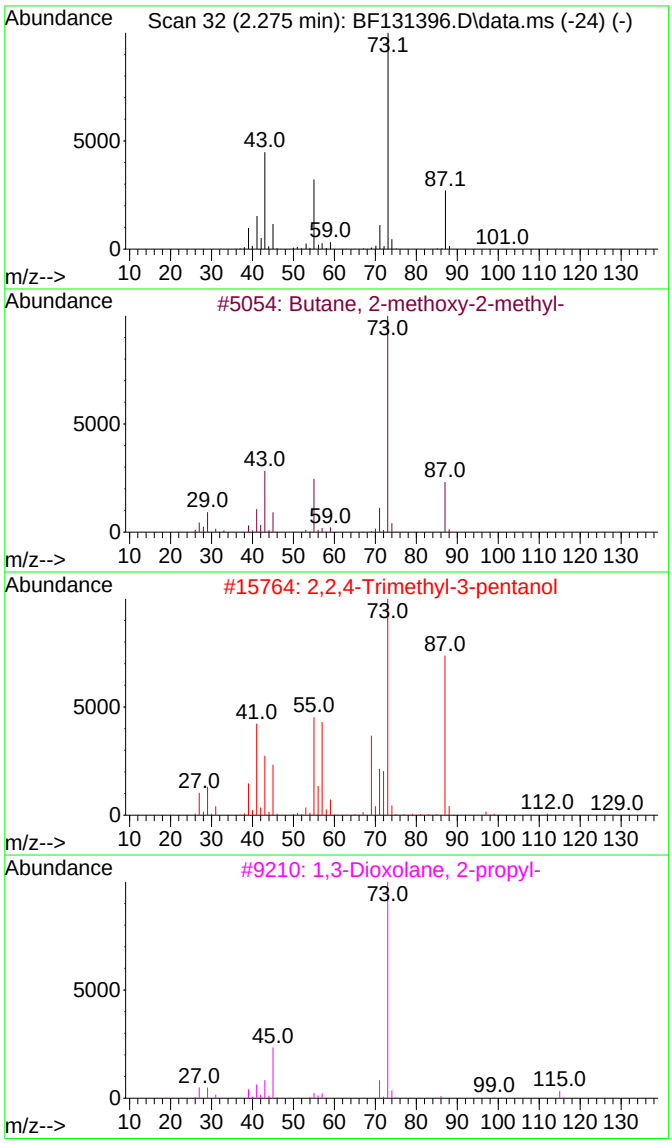
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

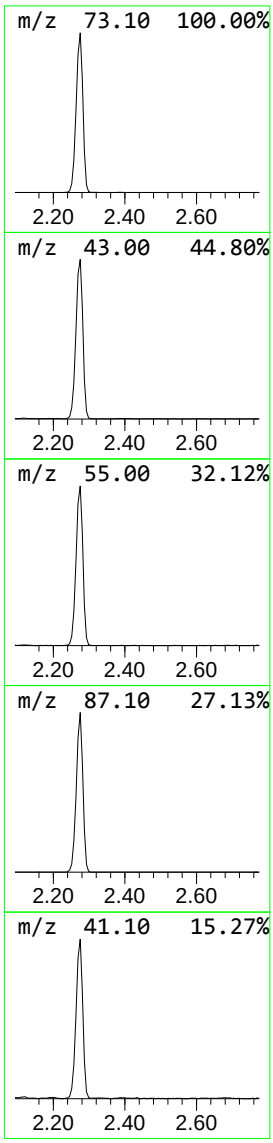
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	70.87 ng	2076900	1,4-Dichlorobenzene-d4	6.957

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-propyl-	116	C6H12O2	003390-13-4	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

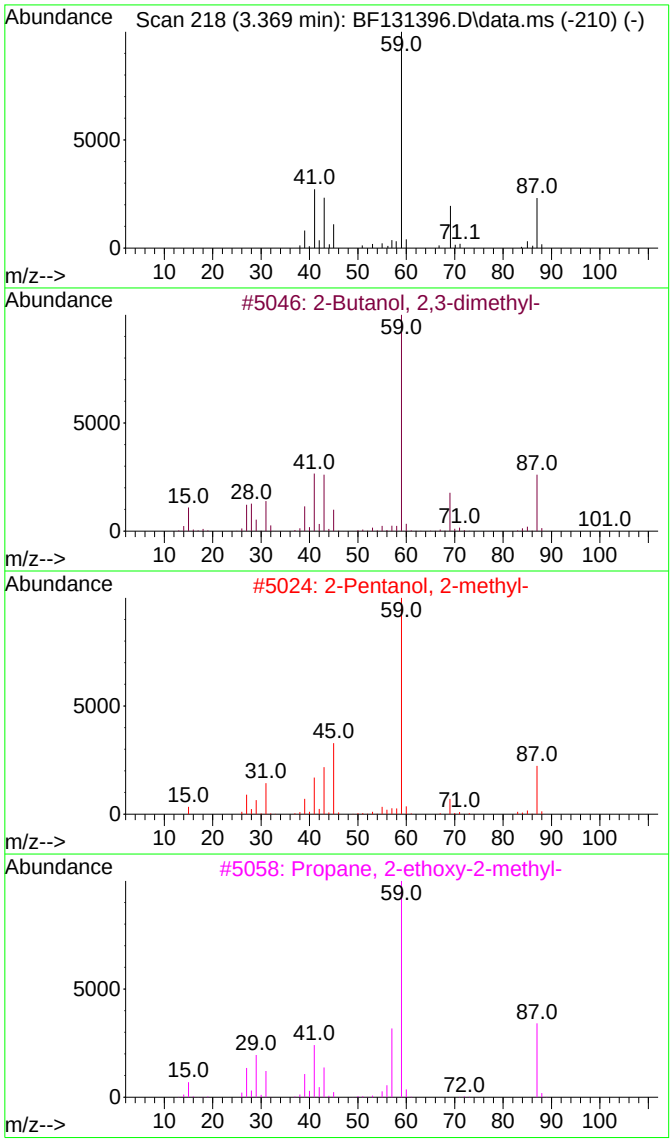
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

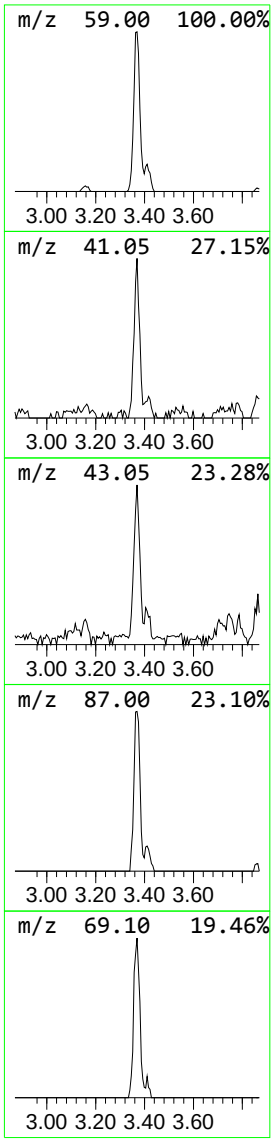
****

Peak Number 2 2-Butanol, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.369	2.96 ng	86816	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	56
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
4	3-Heptanol	116	C7H16O	000589-82-2	40
5	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

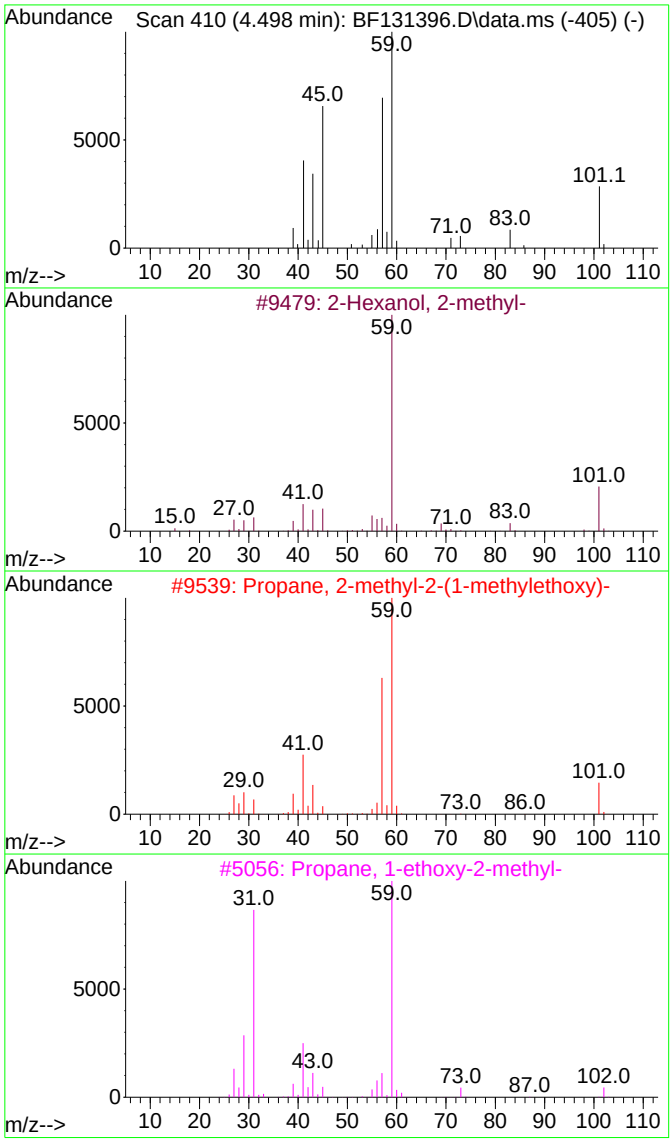
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

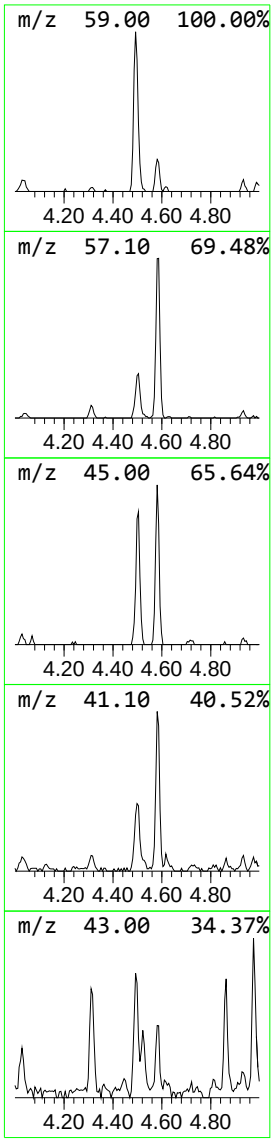
****

Peak Number 3 2-Hexanol, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.498	2.82 ng	82598	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	47
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	47
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

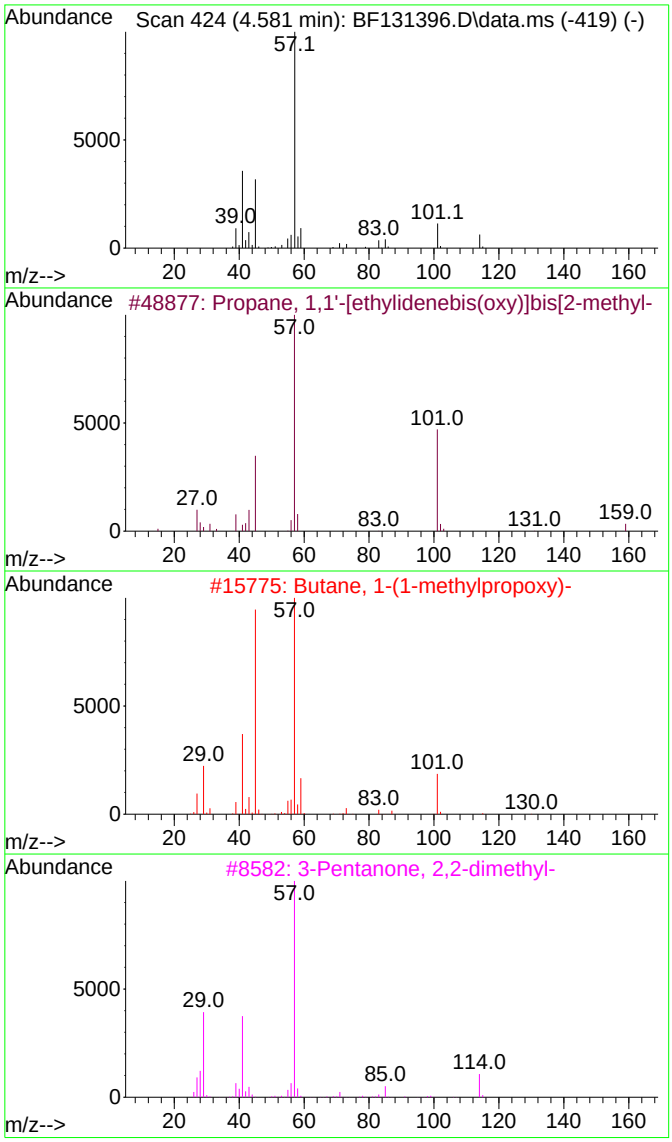
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

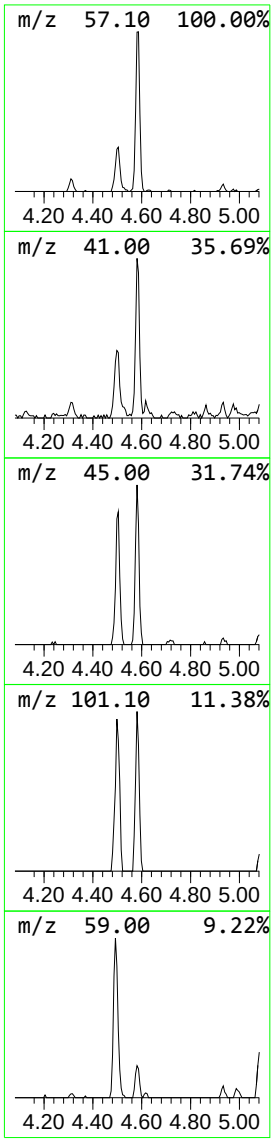
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propane, 1,1'-[ethylidenebi... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.581	3.10 ng	90936	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1'-[ethylidenebis(oxy...	174	C10H22O2	005669-09-0	50
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	45
3	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	38
4	Butanoic acid, 3,3-dimethyl-	116	C6H12O2	001070-83-3	37
5	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131396.D
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Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

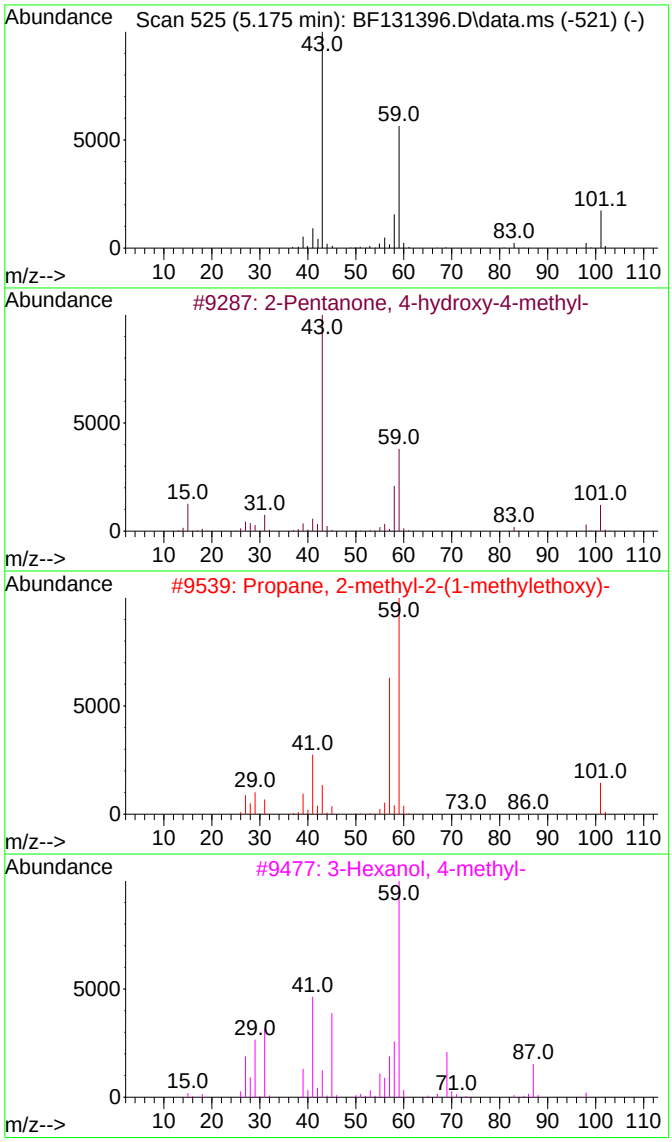
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

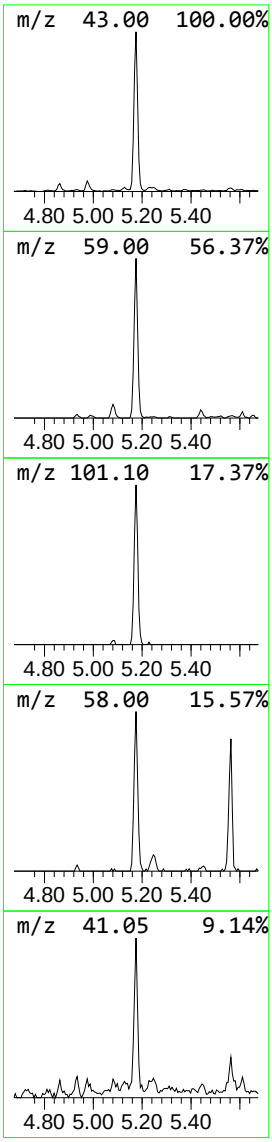
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	7.26 ng	212819	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

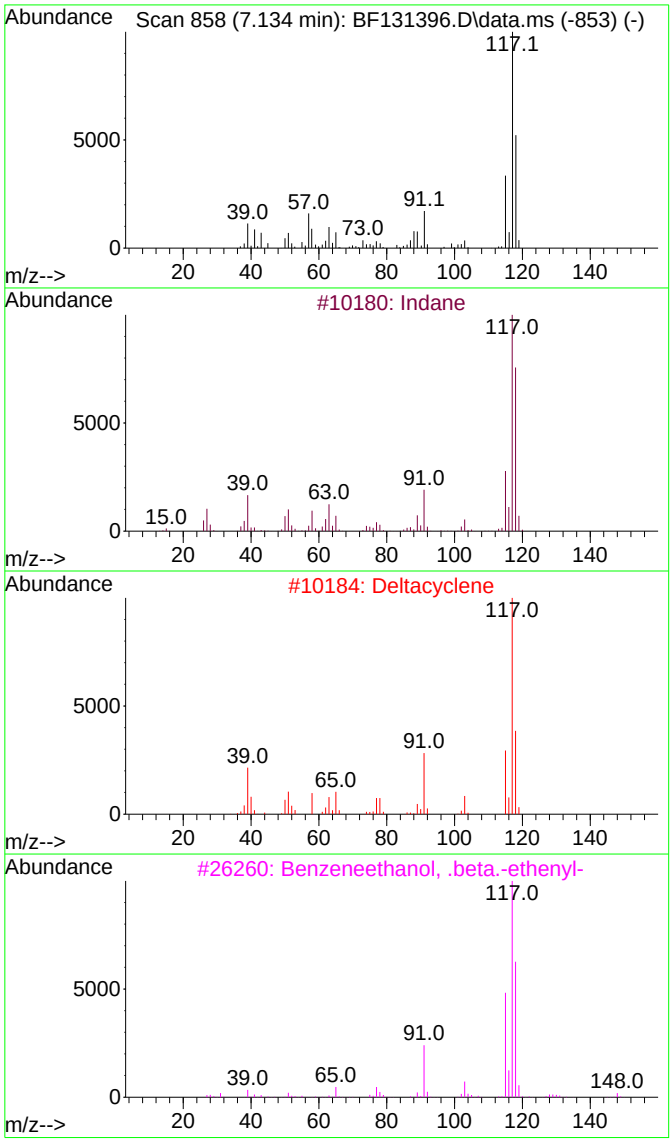
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

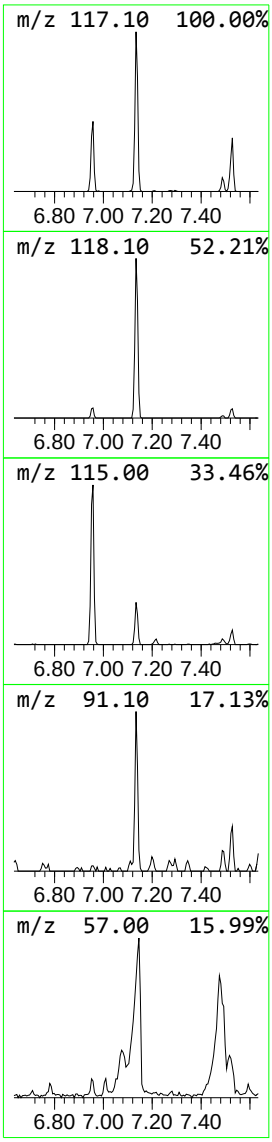
****

Peak Number 6 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.134	8.73 ng	255914	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Deltacyclene	118	C9H10	007785-10-6	64
3	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	53
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	49
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	49





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

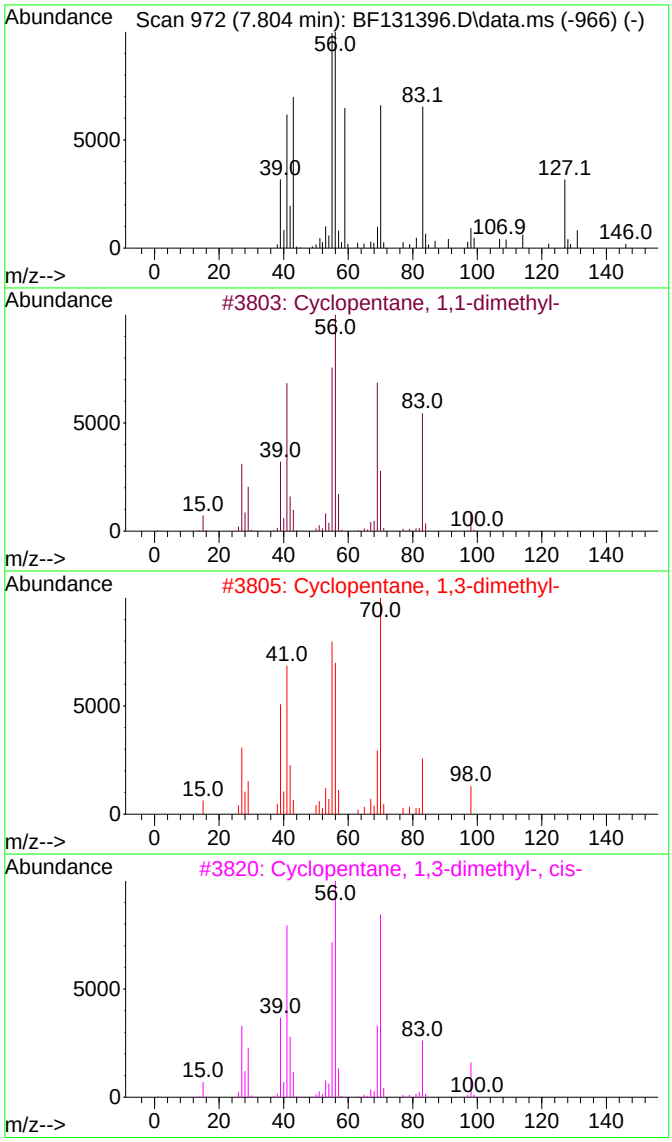
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

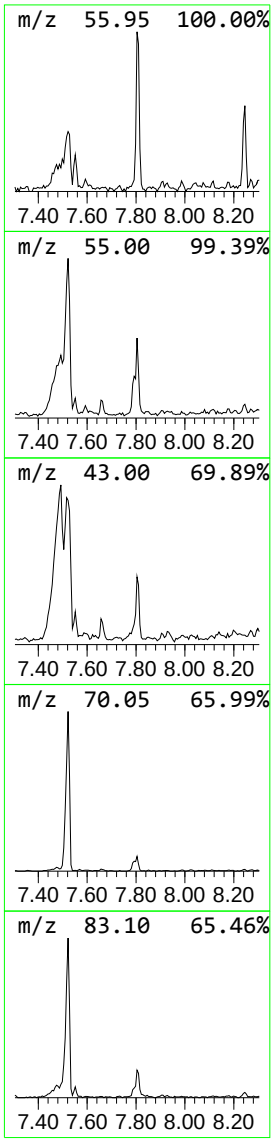
****

Peak Number 7 Cyclopentane, 1,1-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.804	2.84 ng	105540	Naphthalene-d8	8.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	58
2	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	38
3	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	38
4	Isopropylcyclobutane	98	C7H14	000872-56-0	38
5	2-Heptene	98	C7H14	000592-77-8	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

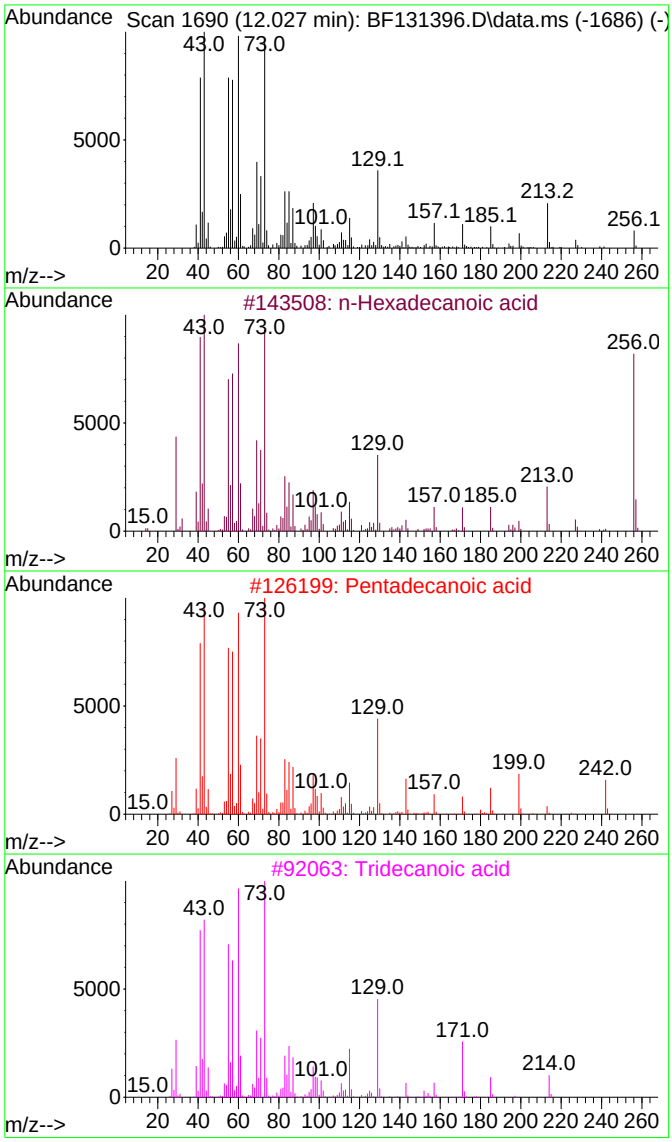
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

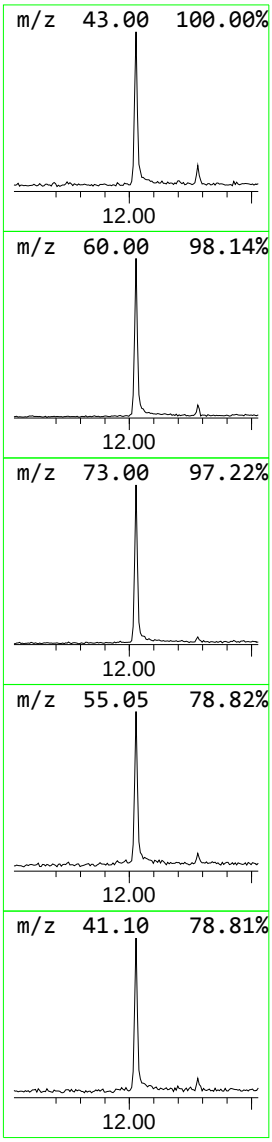
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.027	10.71 ng	426759	Phenanthrene-d10	11.504

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	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131396.D
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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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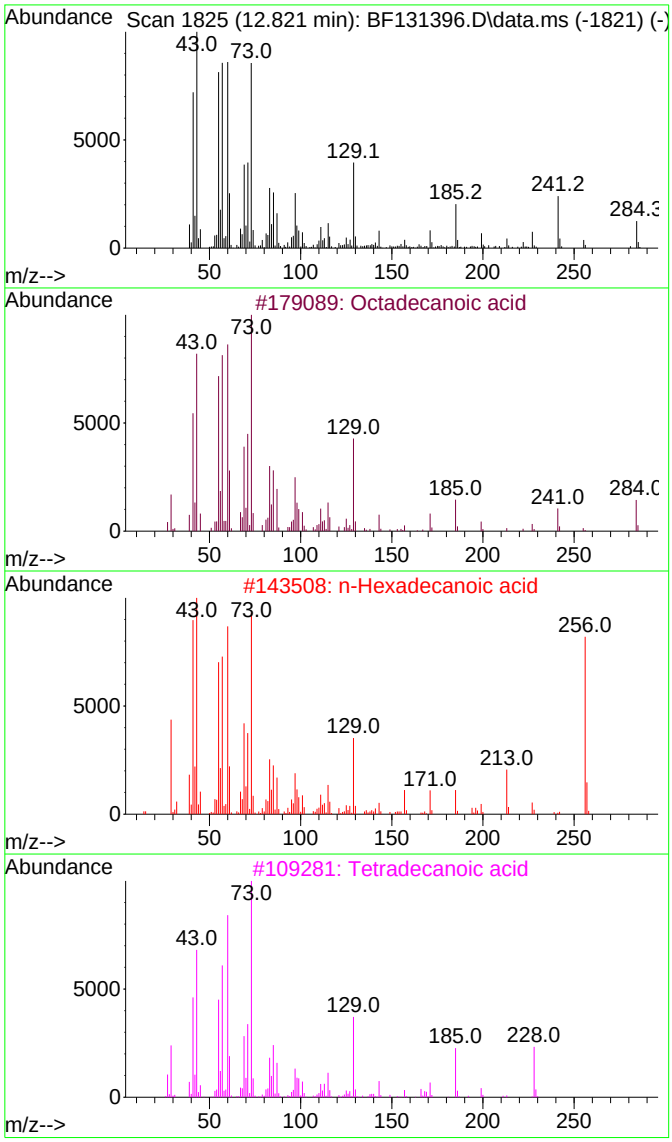
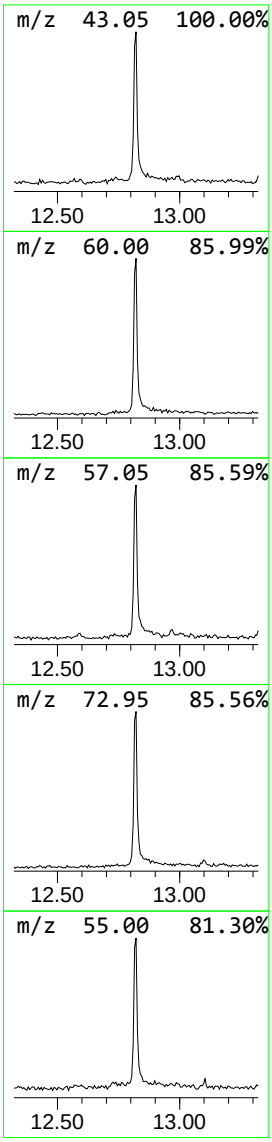
Peak Number 9 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.821	9.15 ng	364426	Phenanthrene-d10	11.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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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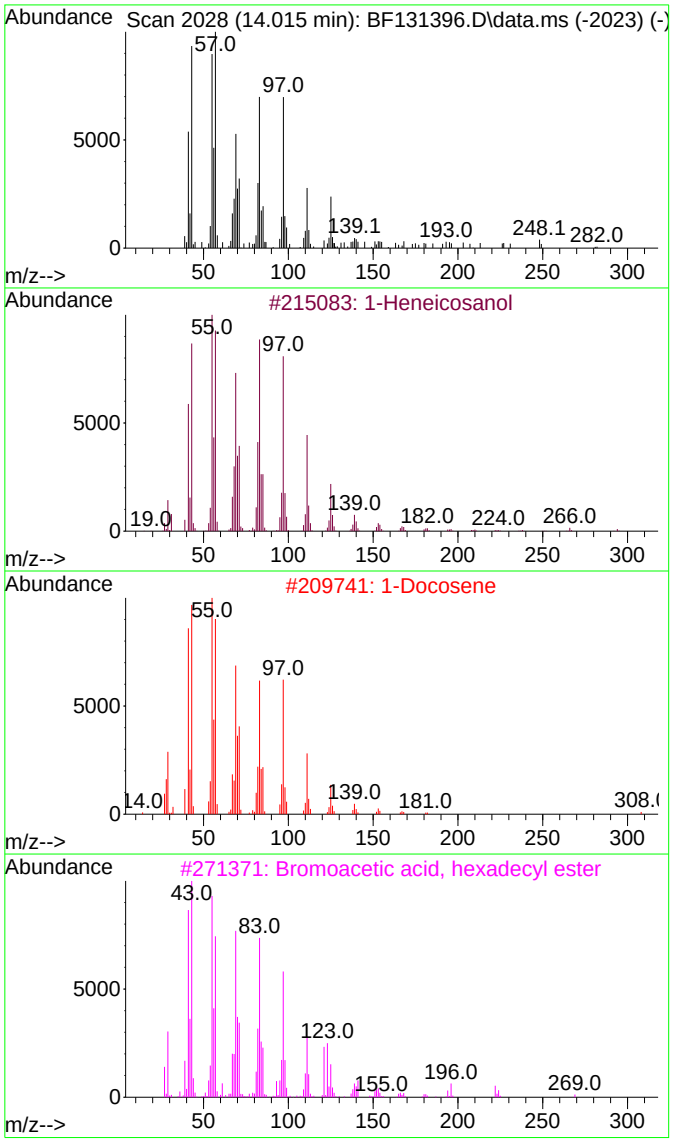
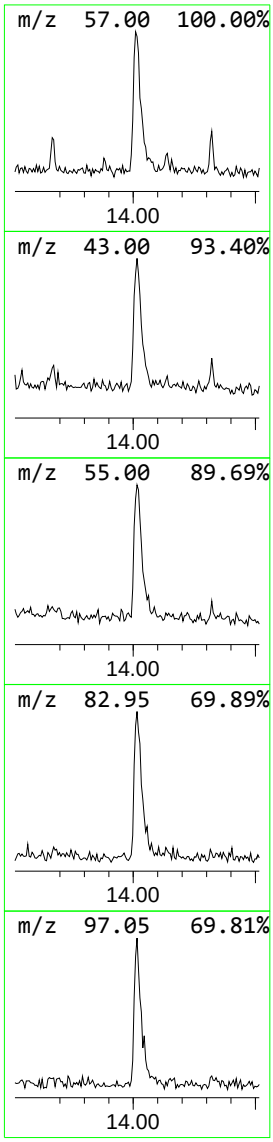
Peak Number 10 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.015	7.78 ng	179439	Chrysene-d12	14.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	1-Docosene	308	C22H44	001599-67-3	90
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	81
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	81
5	Behenic alcohol	326	C22H46O	000661-19-8	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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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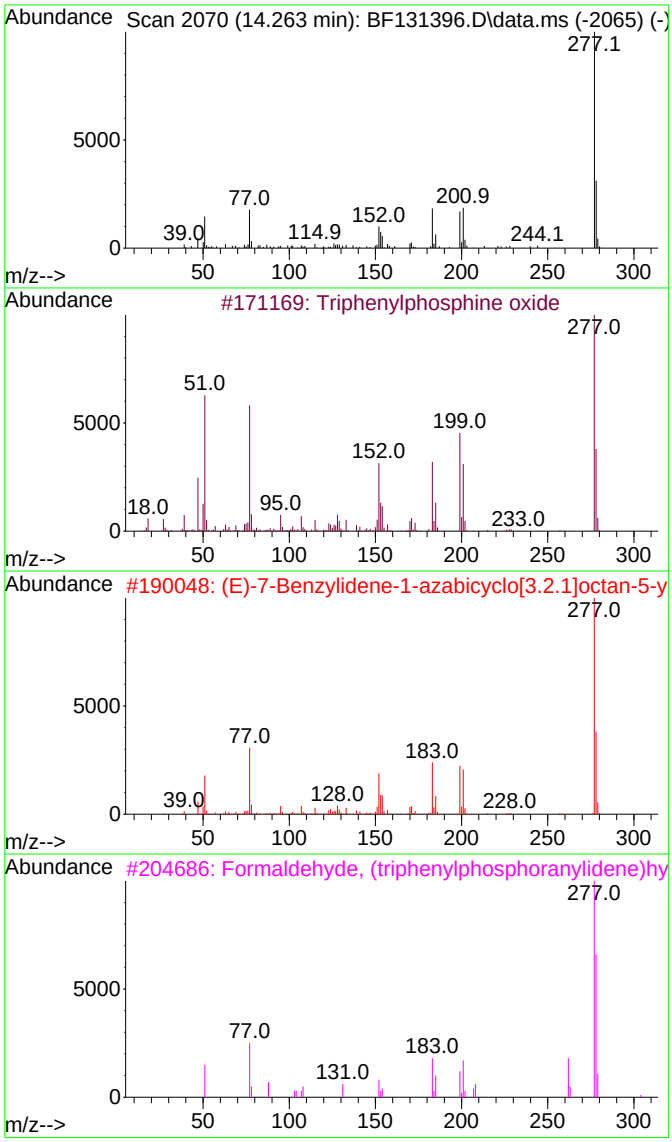
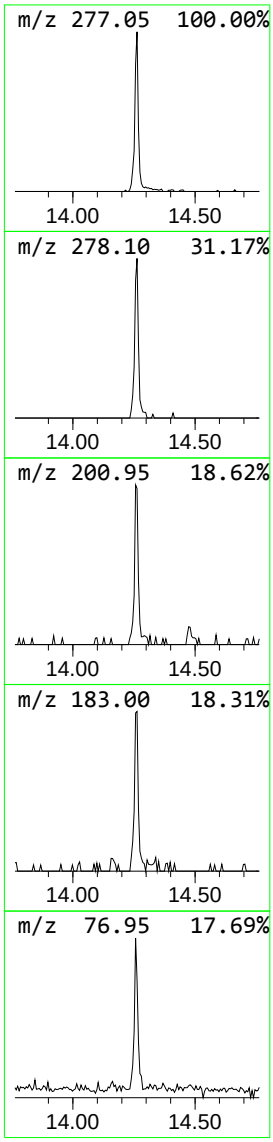
Peak Number 11 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.262	3.36 ng	77540	Chrysene-d12	14.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	83
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	42
5	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131396.D
Acq On : 25 Nov 2022 15:06
Operator : CG\JU
Sample : N5741-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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...	2.275	70.9	ng	2076900	1	6.957	586143	20.0
2-Butanol, 2,3-...	3.369	3.0	ng	86816	1	6.957	586143	20.0
2-Hexanol, 2-me...	4.498	2.8	ng	82598	1	6.957	586143	20.0
Propane, 1,1'-[...	4.581	3.1	ng	90936	1	6.957	586143	20.0
2-Pentanone, 4-...	5.175	7.3	ng	212819	1	6.957	586143	20.0
Indane	7.134	8.7	ng	255914	1	6.957	586143	20.0
Cyclopentane, 1...	7.804	2.8	ng	105540	2	8.245	742020	20.0
n-Hexadecanoic ...	12.027	10.7	ng	426759	4	11.504	796879	20.0
Octadecanoic acid	12.821	9.2	ng	364426	4	11.504	796879	20.0
1-Heneicosanol	14.015	7.8	ng	179439	5	14.163	461287	20.0
Triphenylphosph...	14.262	3.4	ng	77540	5	14.163	461287	20.0