LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
Data File : BF131654.D
Acq On : 15 Dec 2022 17:52
Operator : CG\JU
Sample : N6001-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

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-BF120822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131654.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	12	rVB	1884064	2281943	14.01%	4.890%
2	3.222	188	193	201	rVB	192747	339473	2.08%	0.727%
3	3.710	270	276	284	rVB	268826	401262	2.46%	0.860%
4	3.934	308	314	320	rVB	831504	1101796	6.77%	2.361%
5	4.410	392	395	401	rVB	187548	205375	1.26%	0.440%
6	4.987	488	493	498	rBV	184846	212019	1.30%	0.454%
7	5.098	505	512	515	rBV3	110380	204639	1.26%	0.439%
8	5.134	515	518	528	rVB2	258057	452856	2.78%	0.970%
9	5.369	551	558	561	rBV	6262214	7555791	46.40%	16.192%
10	5.493	569	579	583	rBV	7859851	16284250	100.00%	34.896%
11	5.728	614	619	622	rBV	3472745	3539685	21.74%	7.585%
12	6.504	748	751	756	rBV	855208	713848	4.38%	1.530%
13	6.881	811	815	818	rVB	503288	418581	2.57%	0.897%
14	7.057	842	845	848	rBV	391743	308135	1.89%	0.660%
15	7.287	880	884	886	rBV	227882	194476	1.19%	0.417%
16	7.322	886	890	895	rVB	181699	201325	1.24%	0.431%
17	7.451	899	912	915	rBV	1616084	1763536	10.83%	3.779%
18	7.816	971	974	984	rVB	283158	332213	2.04%	0.712%
19	7.928	984	993	999	rBV	133828	224774	1.38%	0.482%
20	8.169	1030	1034	1037	rVB	635415	536045	3.29%	1.149%
21	9.251	1212	1218	1221	rBV	3388202	2877292	17.67%	6.166%
22	9.933	1329	1334	1337	rBV	699229	634022	3.89%	1.359%
23	10.163	1364	1373	1381	rBV	615659	915071	5.62%	1.961%
24	10.727	1464	1469	1472	rBV	2138643	1790868	11.00%	3.838%
25	11.427	1584	1588	1591	rBV	805616	663203	4.07%	1.421%
26	13.021	1854	1859	1862	rBV	1979556	1711354	10.51%	3.667%
27	14.074	2035	2038	2042	rVB	452726	421984	2.59%	0.904%
28	15.580	2288	2294	2302	rBV	299960	378759	2.33%	0.812%

Sum of corrected areas: 46664575

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
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Operator : CG\JU
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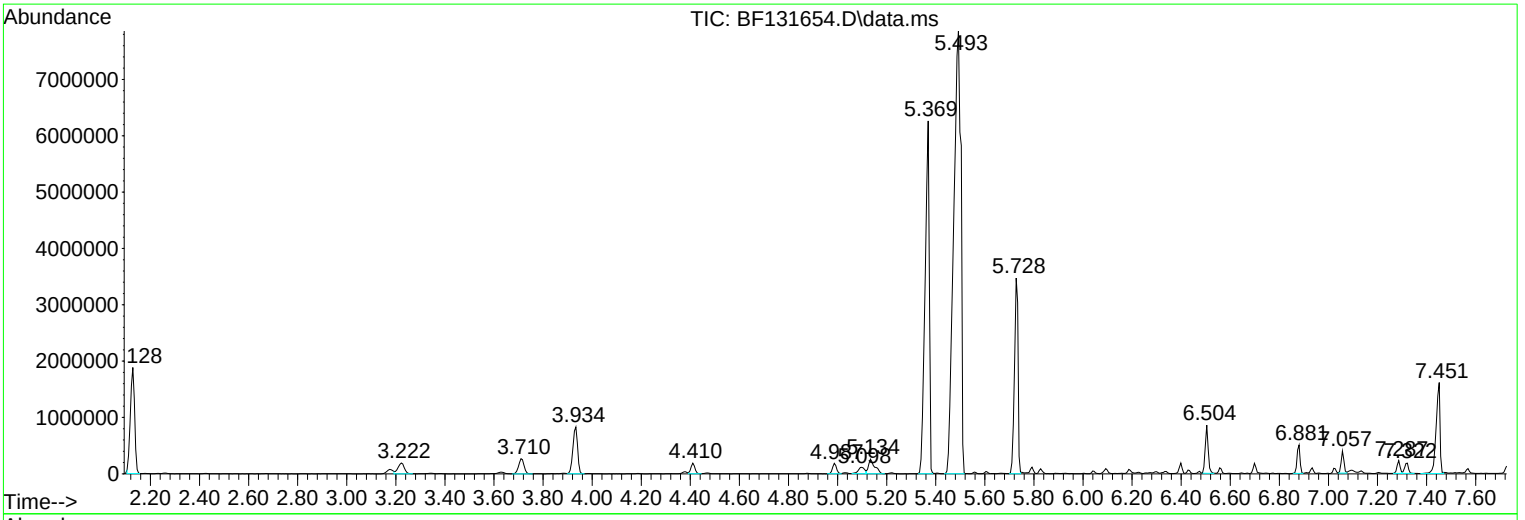
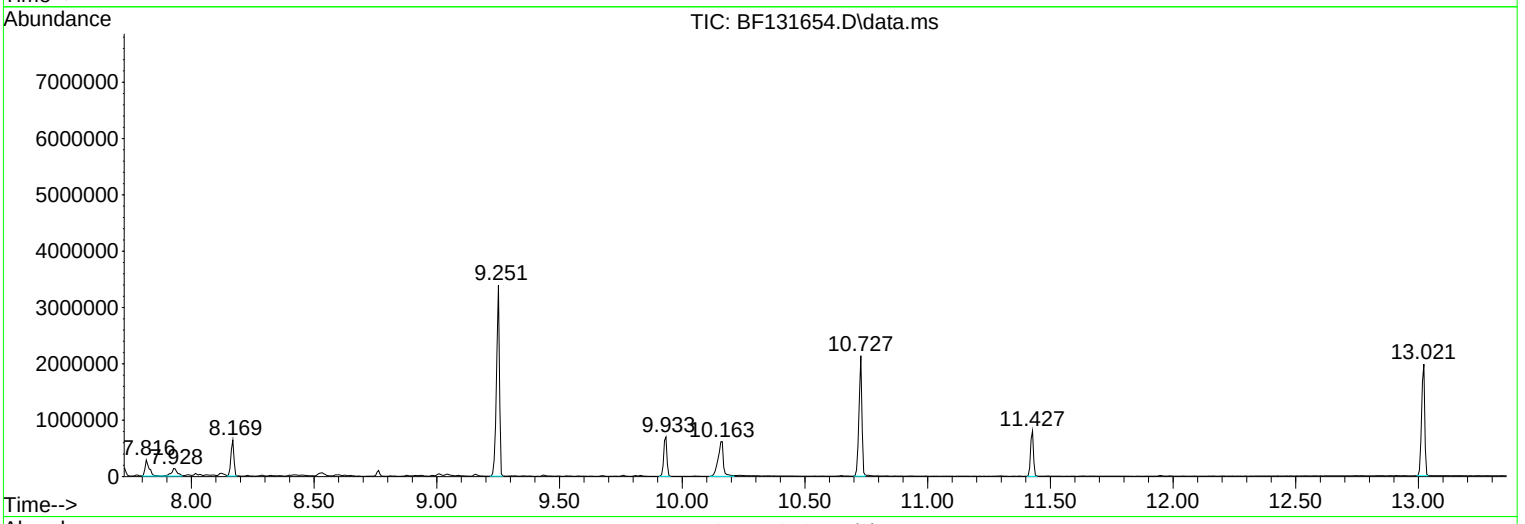
Misc :
ALS Vial : 15 Sample Multiplier: 1

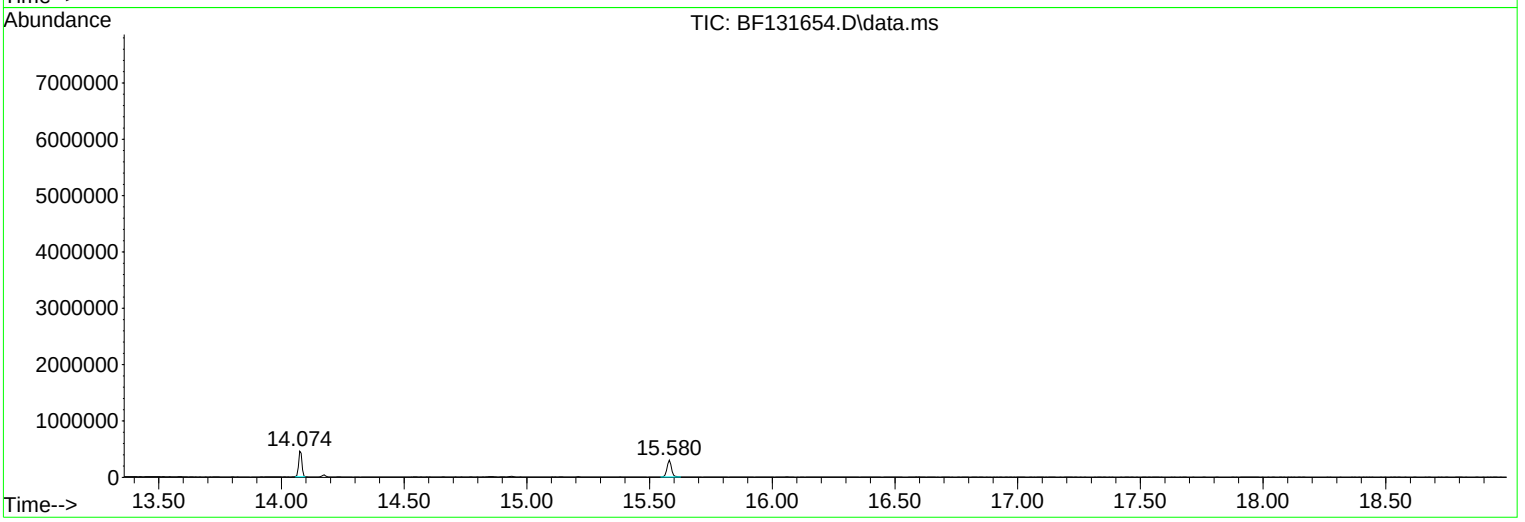
Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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\BF121522\
Data File : BF131654.D
Acq On : 15 Dec 2022 17:52
Operator : CG\JU
Sample : N6001-07
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

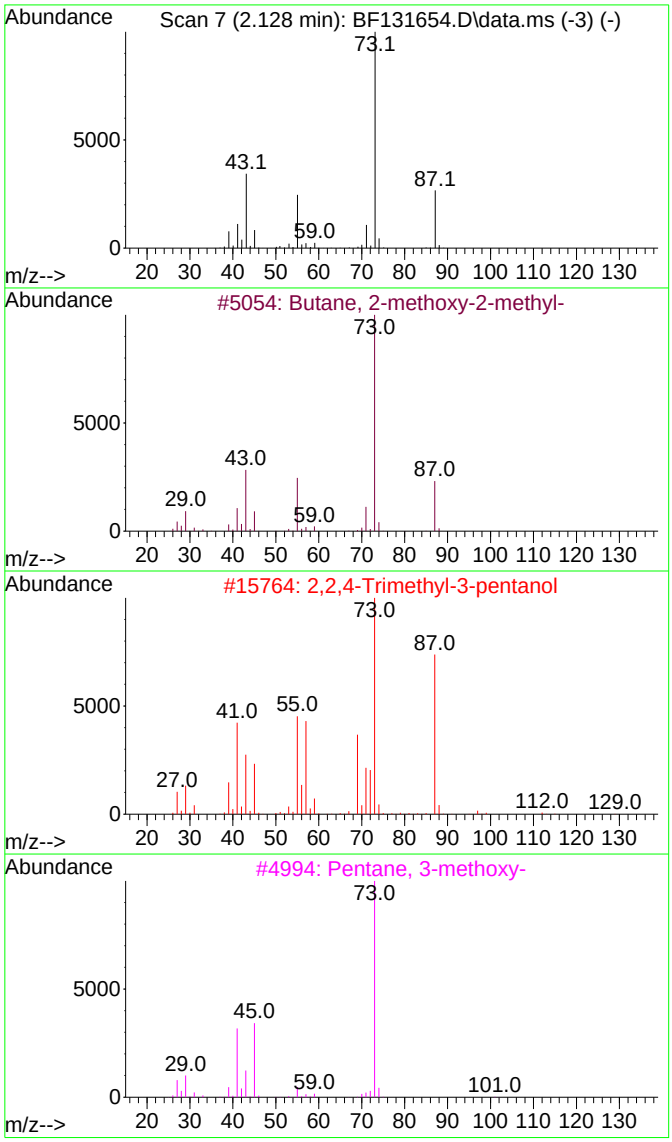
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

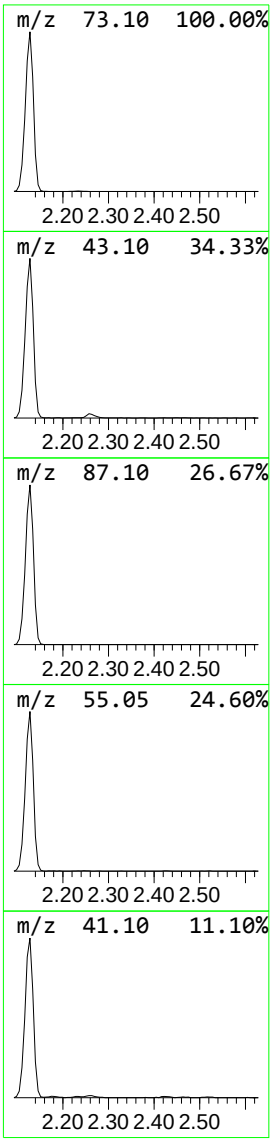
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	109.03 ng	2281940	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
Data File : BF131654.D
Acq On : 15 Dec 2022 17:52
Operator : CG\JU
Sample : N6001-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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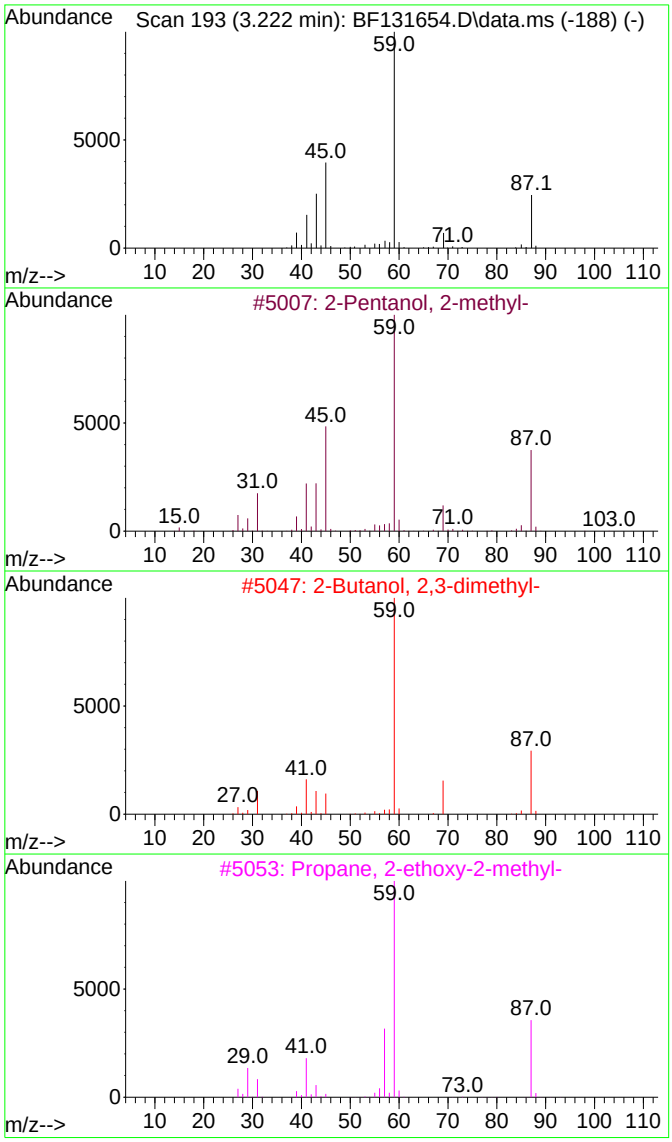
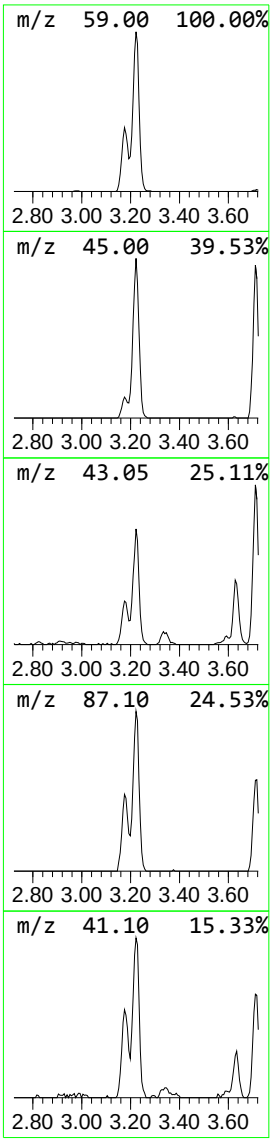
Peak Number 2 2-Pentanol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.222	16.22 ng	339473	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
2	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	42
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	40
4	Amylene hydrate	88	C5H12O	000075-85-4	37
5	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	32





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Data File : BF131654.D
Acq On : 15 Dec 2022 17:52
Operator : CG\JU
Sample : N6001-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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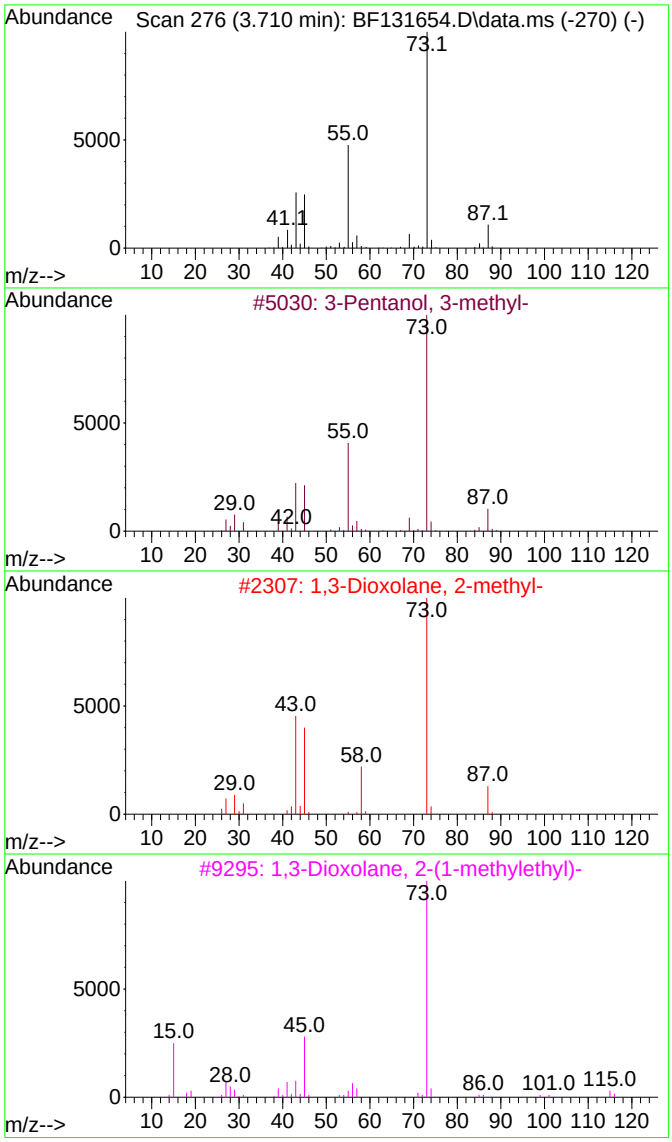
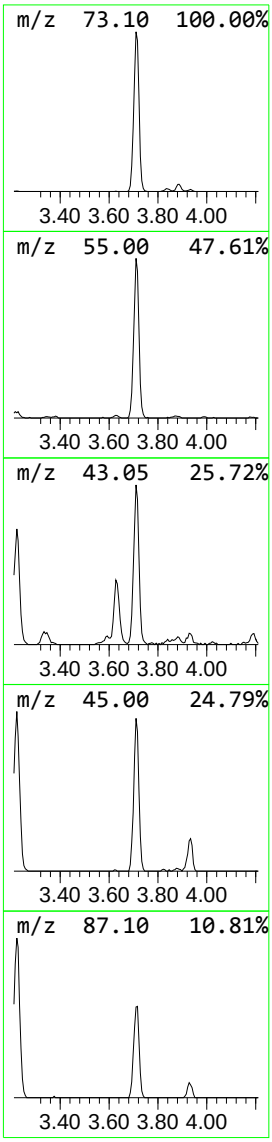
Peak Number 3 3-Pentanol, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.710	19.17 ng	401262	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	78
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	33
4	1,3-Dioxolane, 2-hexyl-	158	C9H18O2	001708-34-5	28
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
Data File : BF131654.D
Acq On : 15 Dec 2022 17:52
Operator : CG\JU
Sample : N6001-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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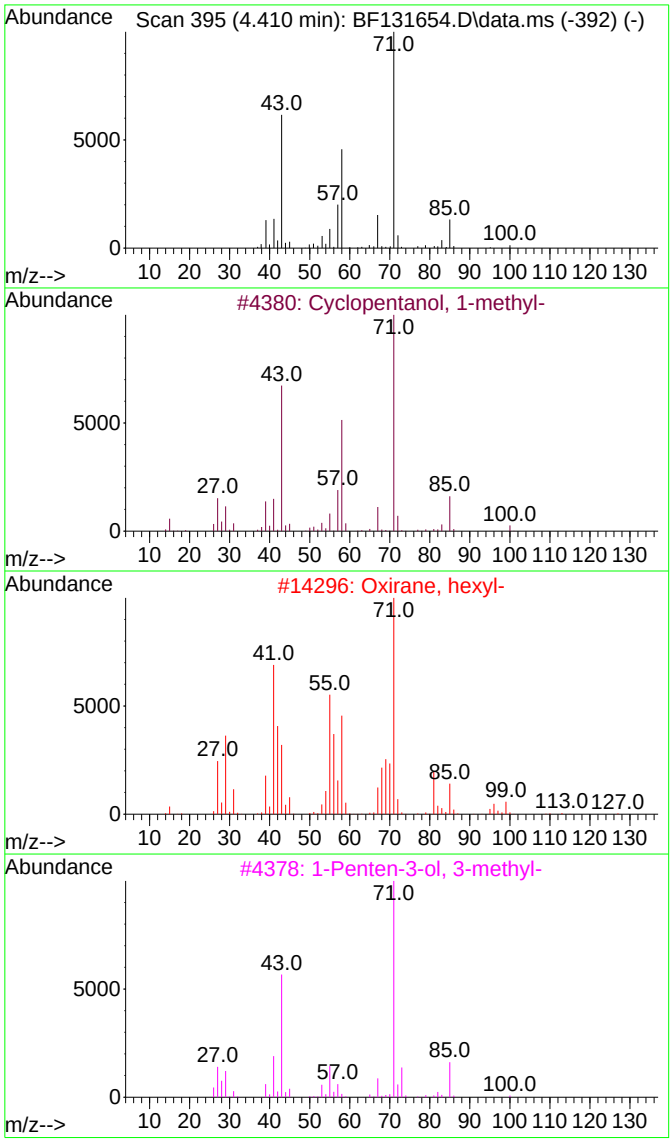
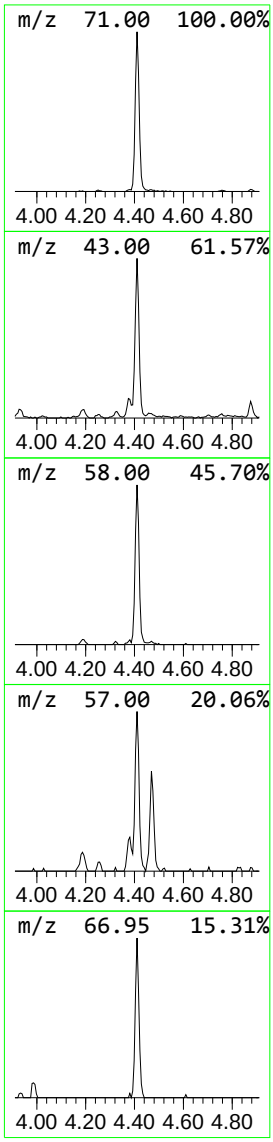
Peak Number 5 Cyclopentanol, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.410	9.81 ng	205375	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanol, 1-methyl-	100	C6H12O	001462-03-9	90
2	Oxirane, hexyl-	128	C8H16O	002984-50-1	43
3	1-Penten-3-ol, 3-methyl-	100	C6H12O	000918-85-4	40
4	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	37
5	Cyclopropanemethanol, .alpha.-bu...	128	C8H16O	004379-16-2	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
Data File : BF131654.D
Acq On : 15 Dec 2022 17:52
Operator : CG\JU
Sample : N6001-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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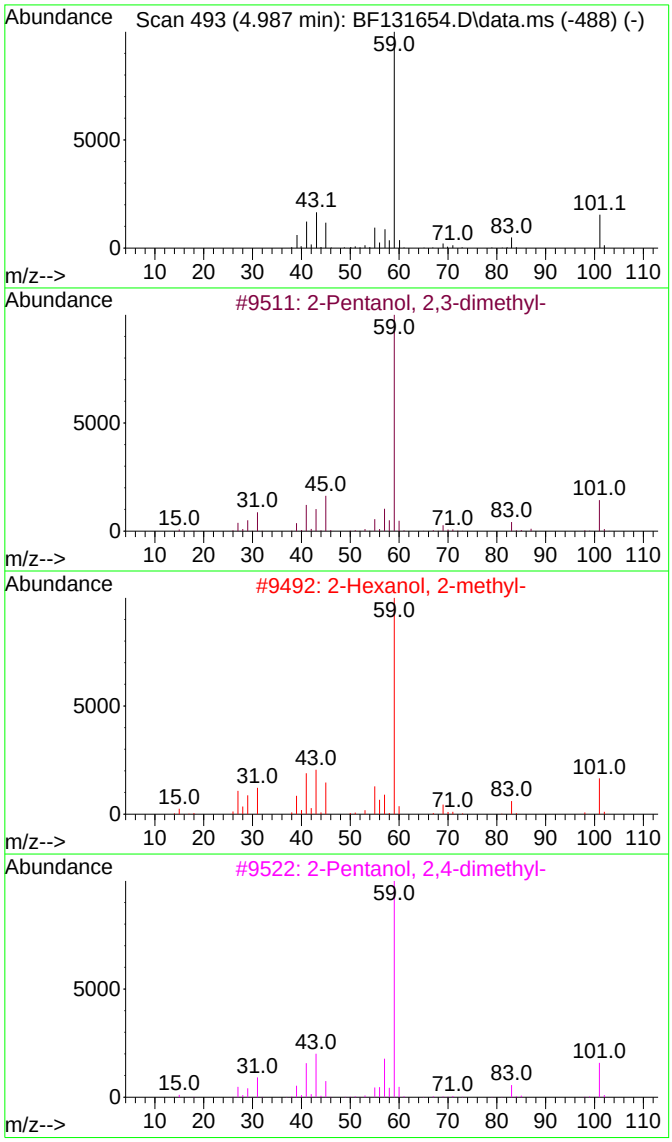
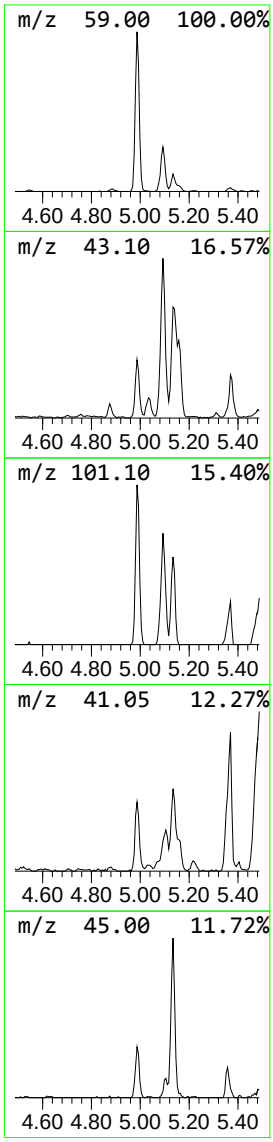
Peak Number 6 2-Pentanol, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	10.13 ng	212019	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	83
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	78
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	64
4	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	56
5	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
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Operator : CG\JU
Sample : N6001-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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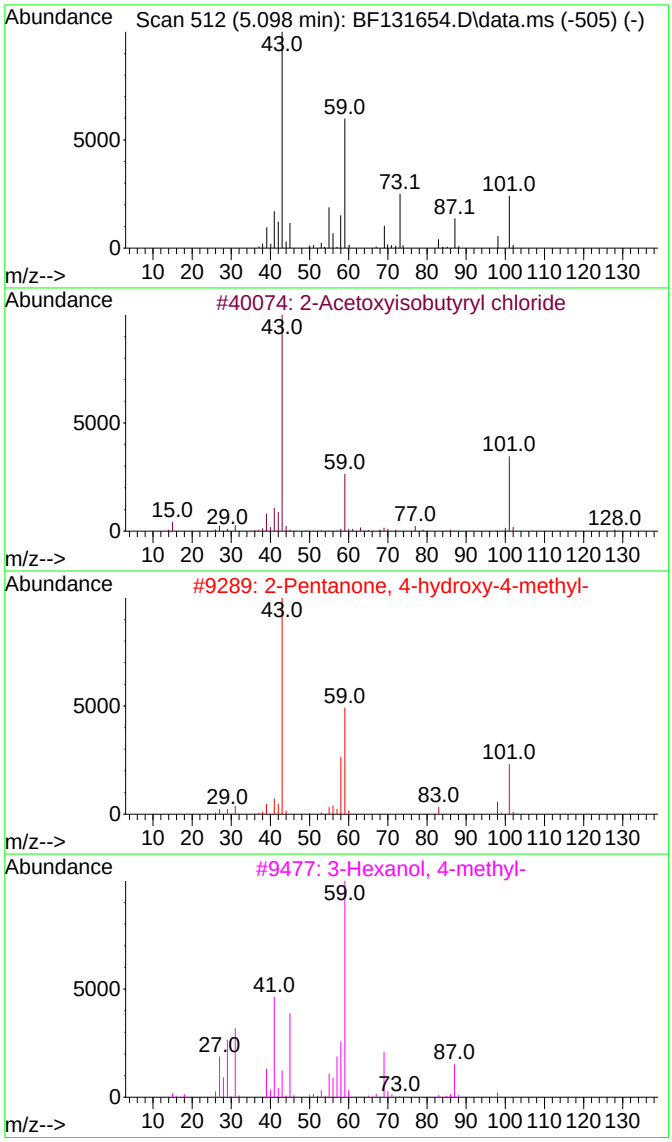
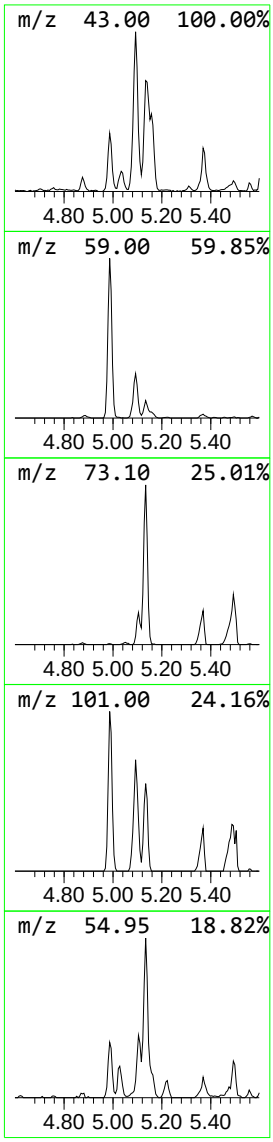
Peak Number 7 unknown5.098 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	9.78 ng	204639	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Acetoxyisobutyryl chloride	164	C6H9ClO3	040635-66-3	47
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	37
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	32
4	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	30
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25





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Data File : BF131654.D
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Operator : CG\JU
Sample : N6001-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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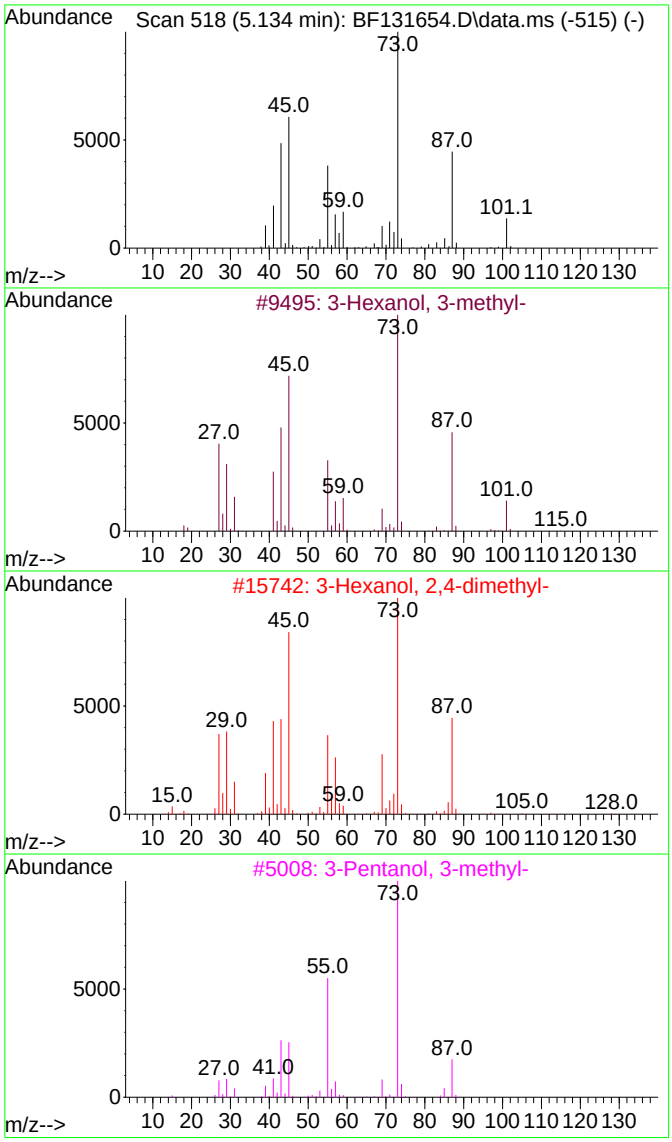
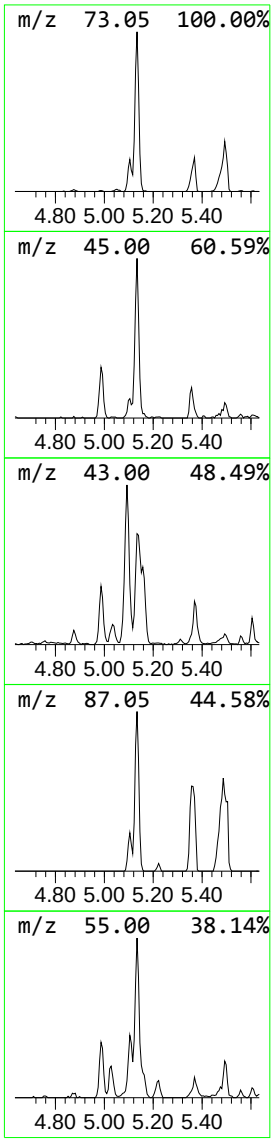
Peak Number 8 3-Hexanol, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	21.64 ng	452856	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	86
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	53
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	40
4	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	40
5	4-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-79-2	38





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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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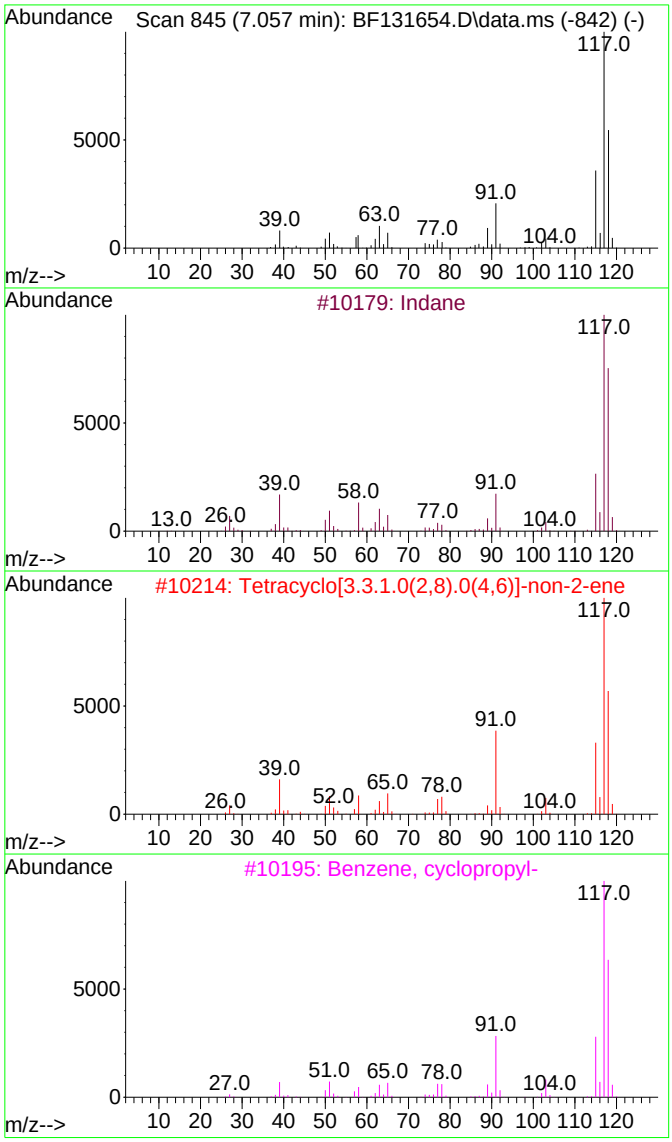
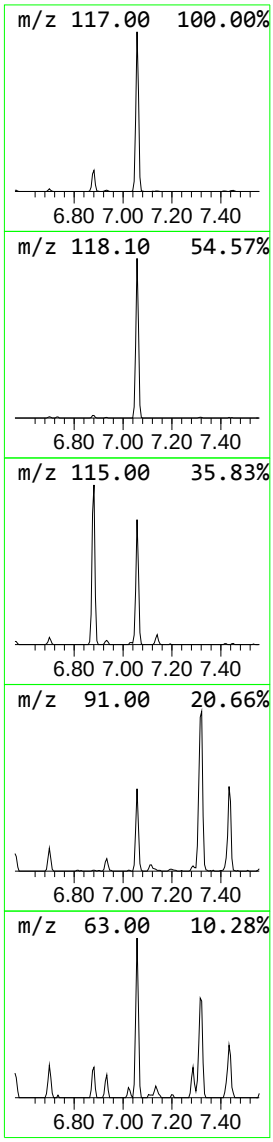
Peak Number 11 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.057	14.72 ng	308135	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	53
5	Indole	117	C8H7N	000120-72-9	52





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Data File : BF131654.D
Acq On : 15 Dec 2022 17:52
Operator : CG\JU
Sample : N6001-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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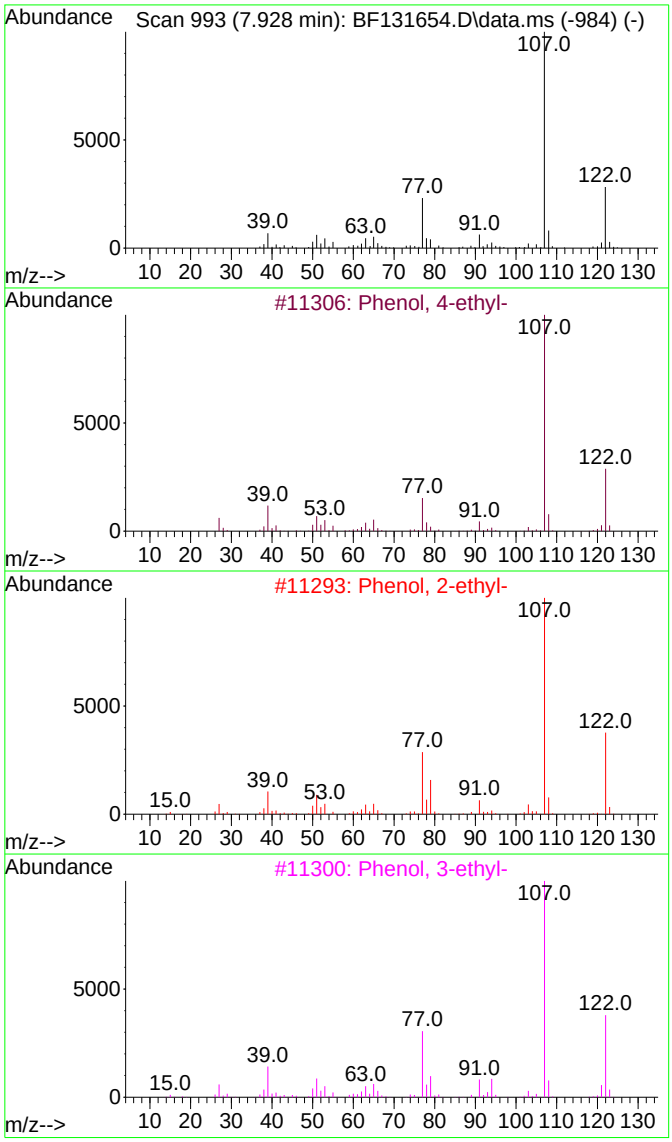
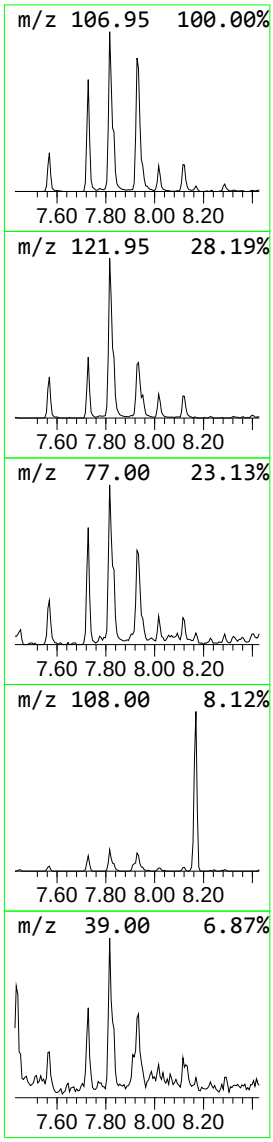
Peak Number 12 Phenol, 4-ethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.928	8.39 ng	224774	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	93
2	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	91
3	Phenol, 3-ethyl-	122	C8H10O	000620-17-7	91
4	Phenol, 3,4-dimethyl-	122	C8H10O	000095-65-8	78
5	1,3-Cyclopentadiene, 5,5-dimethy...	122	C9H14	1000162-25-6	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
Data File : BF131654.D
Acq On : 15 Dec 2022 17:52
Operator : CG\JU
Sample : N6001-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

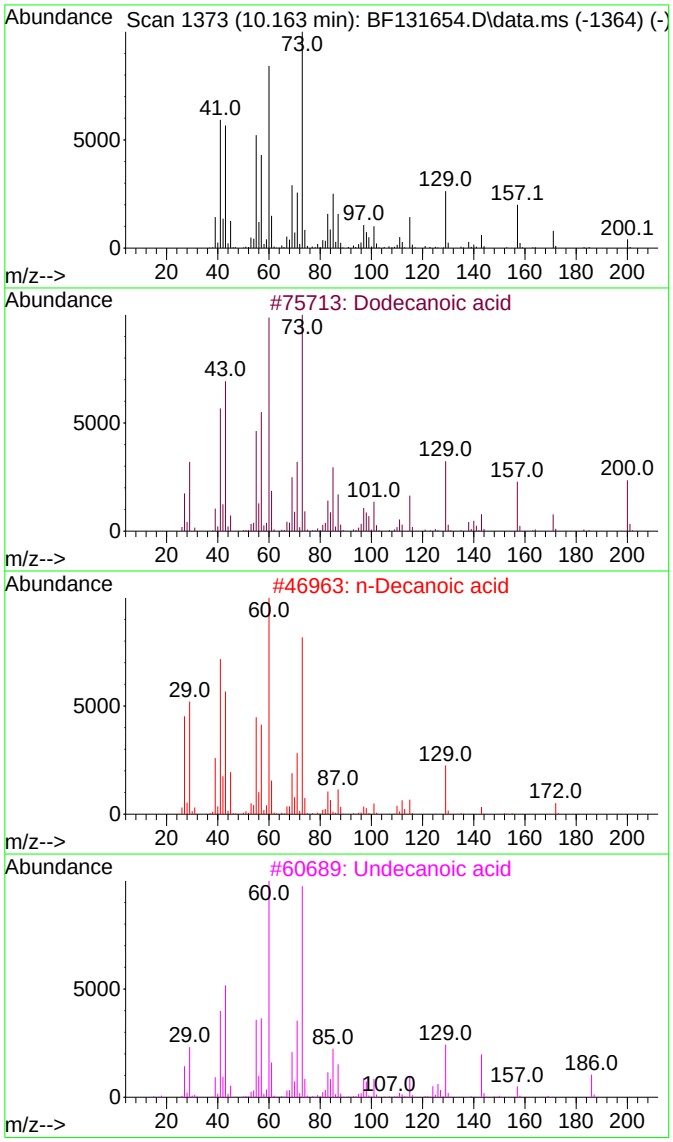
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

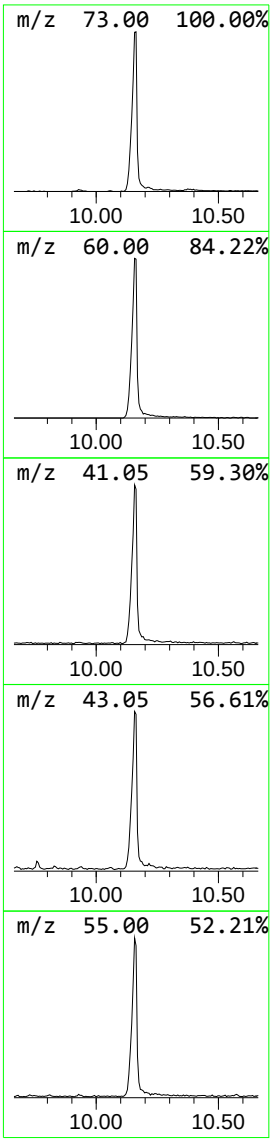
****

Peak Number 13 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.163	28.87 ng	915071	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	94
2	n-Decanoic acid	172	C10H20O2	000334-48-5	81
3	Undecanoic acid	186	C11H22O2	000112-37-8	80
4	Nonanoic acid	158	C9H18O2	000112-05-0	52
5	Octanoic acid	144	C8H16O2	000124-07-2	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
Data File : BF131654.D
Acq On : 15 Dec 2022 17:52
Operator : CG\JU
Sample : N6001-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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...	2.128	109.0	ng	2281940	1	6.881	418581	20.0
2-Pentanol, 2-m...	3.222	16.2	ng	339473	1	6.881	418581	20.0
3-Pentanol, 3-m...	3.710	19.2	ng	401262	1	6.881	418581	20.0
Cyclopentanol, ...	4.410	9.8	ng	205375	1	6.881	418581	20.0
2-Pentanol, 2,3...	4.987	10.1	ng	212019	1	6.881	418581	20.0
unknown5.098	5.098	9.8	ng	204639	1	6.881	418581	20.0
3-Hexanol, 3-me...	5.134	21.6	ng	452856	1	6.881	418581	20.0
Indane	7.057	14.7	ng	308135	1	6.881	418581	20.0
Phenol, 4-ethyl-	7.928	8.4	ng	224774	2	8.169	536045	20.0
Dodecanoic acid	10.163	28.9	ng	915071	3	9.933	634022	20.0