LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130197.D
Acq On : 09 Sep 2022 16:26
Operator : CG\JU
Sample : N4549-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-55

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-BF083122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130197.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.228	145	160	166	rBV2	47482	123098	2.54%	0.398%
2	3.387	174	187	194	rBV	74663	163584	3.38%	0.529%
3	4.392	352	358	367	rBV	72939	108676	2.24%	0.351%
4	4.875	436	440	446	rBV	148282	178683	3.69%	0.578%
5	5.292	507	511	514	rBV	2177613	1918690	39.60%	6.202%
6	6.322	681	686	690	rBV	1378631	1338064	27.61%	4.325%
7	6.634	735	739	740	rBV	86571	78531	1.62%	0.254%
8	6.692	745	749	752	rBV	1306366	1001573	20.67%	3.238%
9	6.945	788	792	795	rBV	302859	243577	5.03%	0.787%
10	7.033	805	807	811	rVB	78623	60721	1.25%	0.196%
11	7.169	826	830	833	rVB2	57974	60665	1.25%	0.196%
12	7.233	836	841	842	rBV	352937	360406	7.44%	1.165%
13	7.257	842	845	848	rVB	2971906	3081122	63.59%	9.960%
14	7.339	855	859	863	rBV2	90345	93502	1.93%	0.302%
15	7.381	863	866	870	rVV2	72435	71577	1.48%	0.231%
16	7.463	873	880	884	rBV	519455	433883	8.95%	1.403%
17	7.710	918	922	926	rVB2	113974	114304	2.36%	0.370%
18	7.892	949	953	960	rBV2	93721	219076	4.52%	0.708%
19	7.975	961	967	969	rVV	1639032	1474903	30.44%	4.768%
20	7.992	969	970	973	rVV2	165773	119510	2.47%	0.386%
21	8.022	973	975	979	rVB	97366	80569	1.66%	0.260%
22	8.357	1029	1032	1035	rBV2	73820	71608	1.48%	0.231%
23	8.533	1059	1062	1064	rBV	91938	70354	1.45%	0.227%
24	9.051	1145	1150	1153	rBV	5370049	4845622	100.00%	15.664%
25	9.722	1258	1264	1268	rBV	1724049	1406316	29.02%	4.546%
26	9.933	1296	1300	1303	rBV2	47536	52834	1.09%	0.171%
27	10.427	1381	1384	1389	rBV3	41578	58410	1.21%	0.189%
28	10.510	1393	1398	1401	rBV	3072575	2699037	55.70%	8.725%
29	11.204	1512	1516	1519	rBV	1326287	1171771	24.18%	3.788%
30	11.739	1603	1607	1616	rBV	609087	639395	13.20%	2.067%
31	12.445	1722	1727	1732	rBV4	67888	142366	2.94%	0.460%
32	12.533	1735	1742	1756	rVV	2019467	2277912	47.01%	7.364%
33	12.792	1781	1786	1789	rBV	4837673	4230817	87.31%	13.677%
34	13.245	1860	1863	1872	rBV10	22358	53829	1.11%	0.174%
35	13.833	1959	1963	1966	rBV	894556	838907	17.31%	2.712%
36	15.233	2196	2201	2206	rBV	882666	1050523	21.68%	3.396%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130197.D
Acq On : 09 Sep 2022 16:26
Operator : CG\JU
Sample : N4549-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-55

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-BF083122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

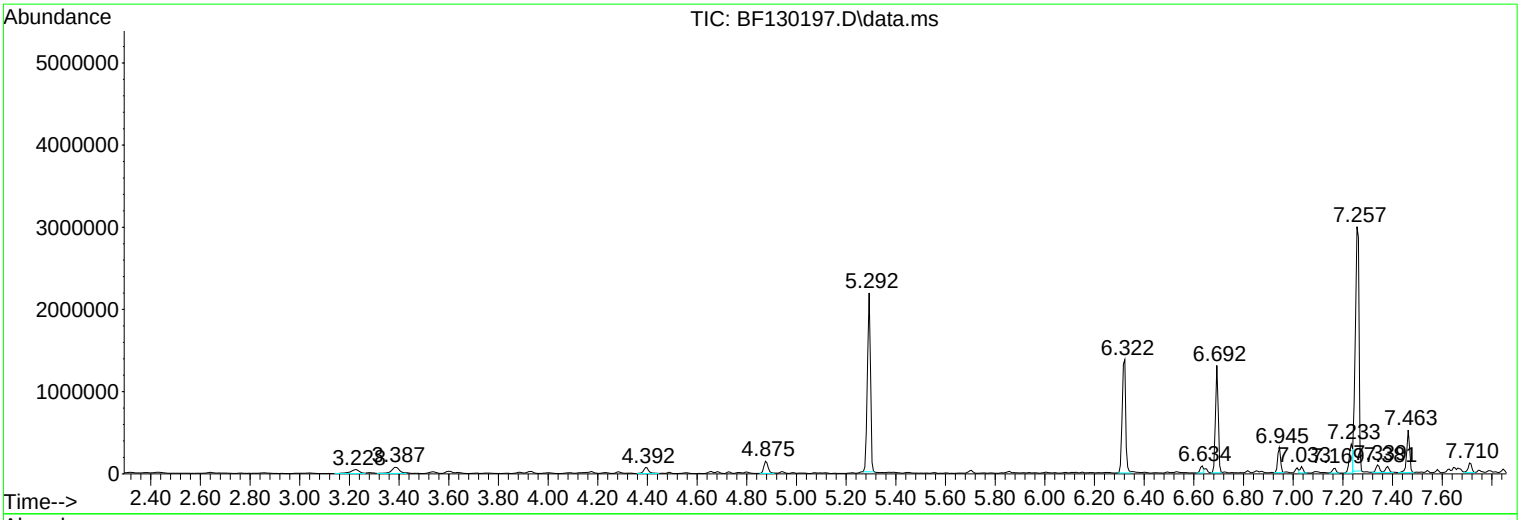
Sum of corrected areas: 30934415

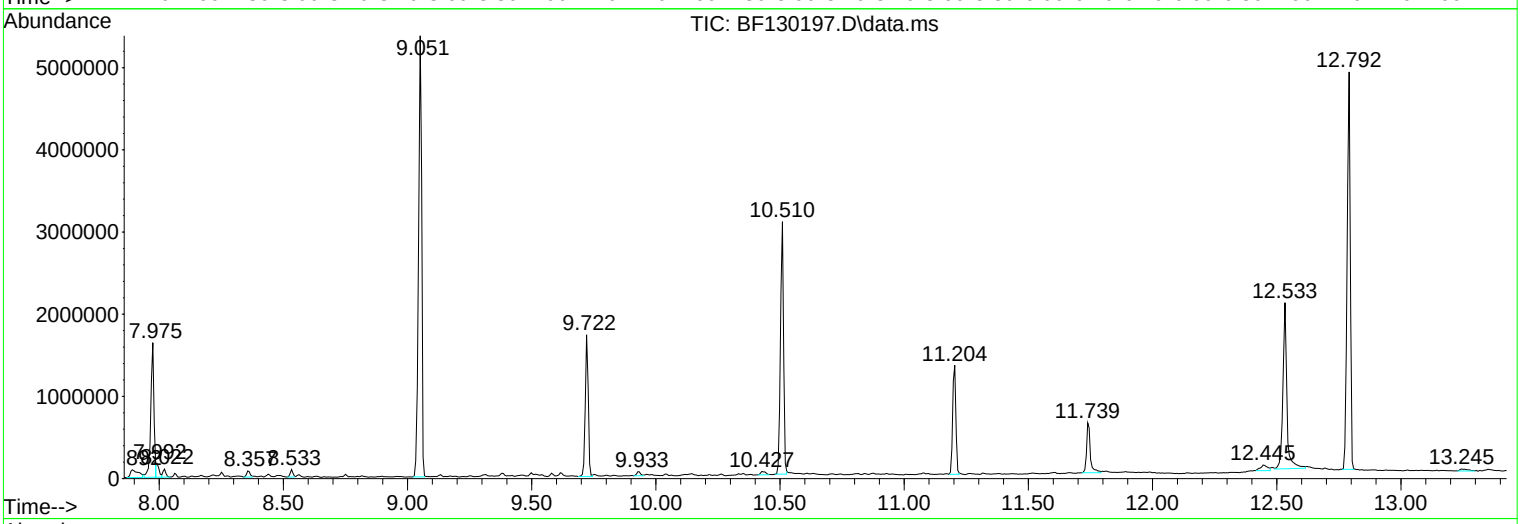
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130197.D
Acq On : 09 Sep 2022 16:26
Operator : CG\JU
Sample : N4549-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

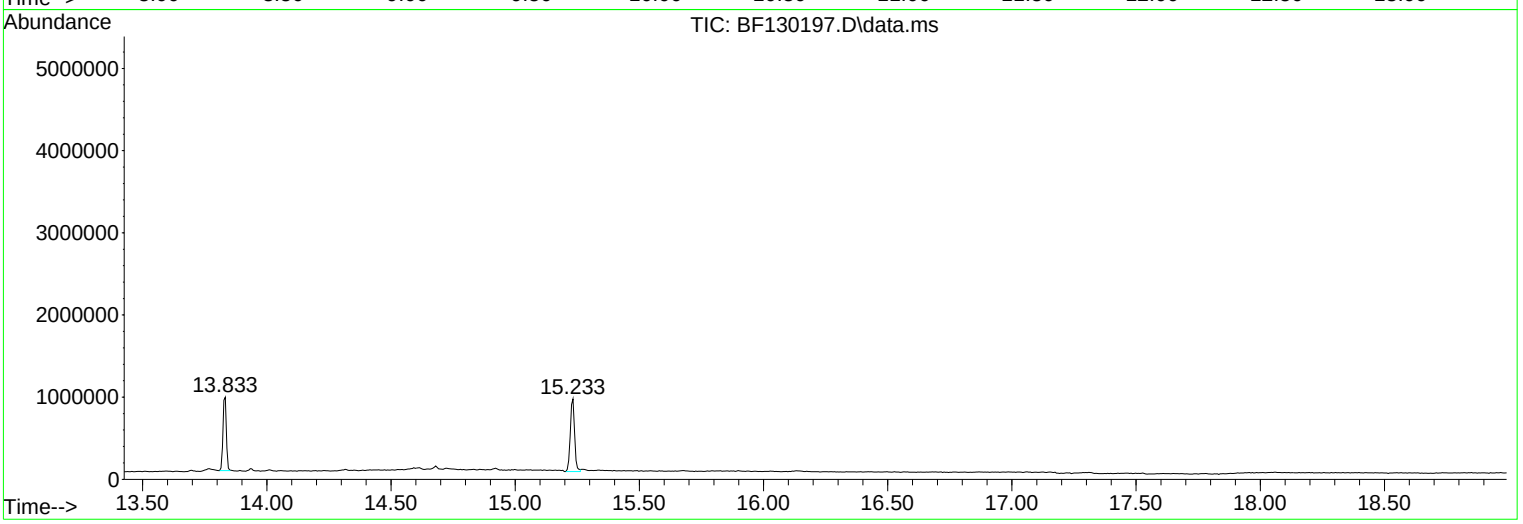
Instrument :
BNA_F
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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\BF090922\
Data File : BF130197.D
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Sample : N4549-11
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

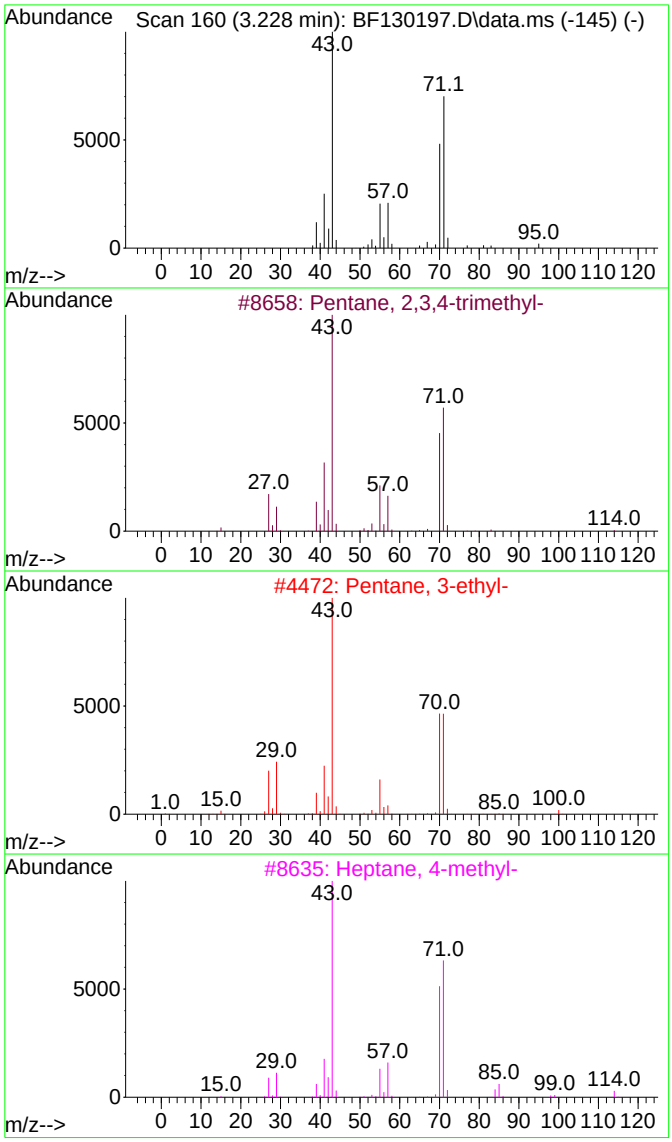
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

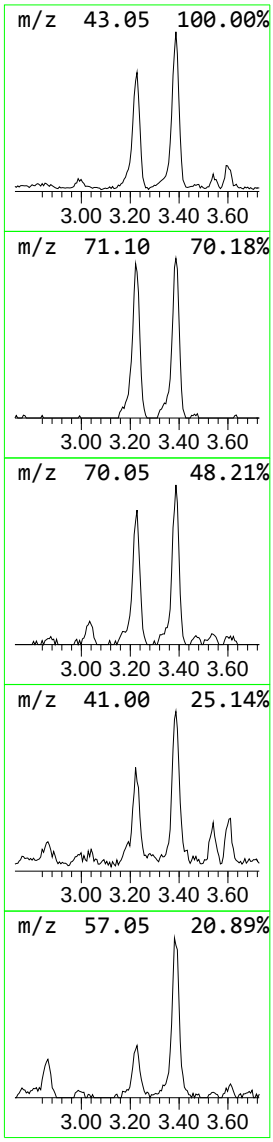
****

Peak Number 1 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.228	2.46 ng	123098	1,4-Dichlorobenzene-d4	6.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	74
4	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	50
5	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	50





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Data File : BF130197.D
Acq On : 09 Sep 2022 16:26
Operator : CG\JU
Sample : N4549-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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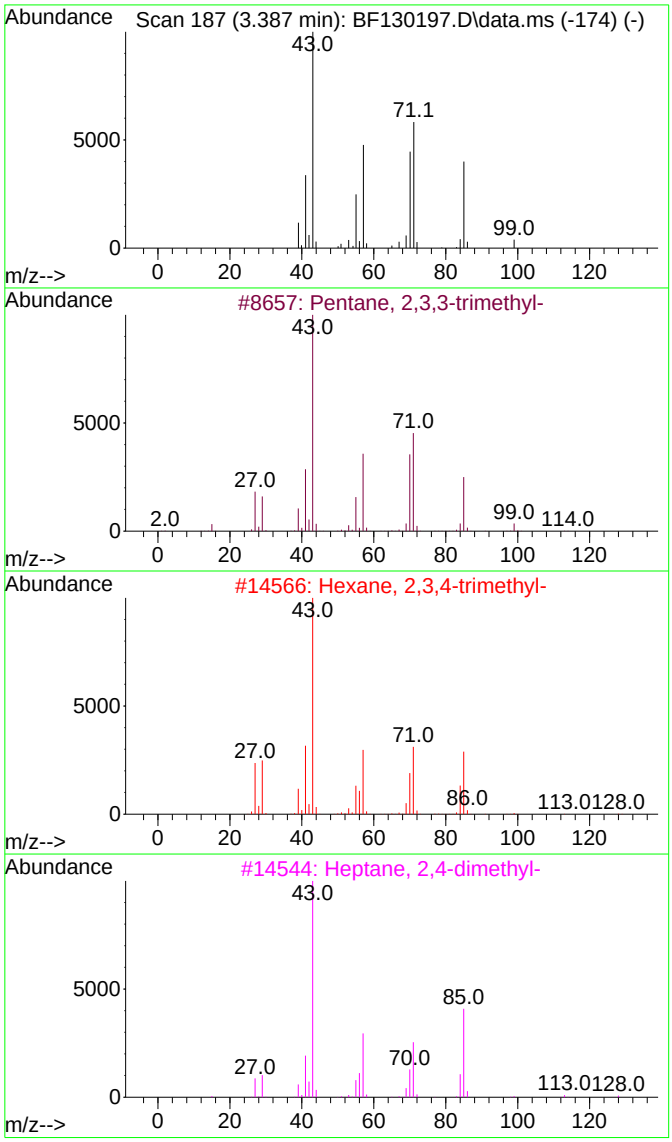
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

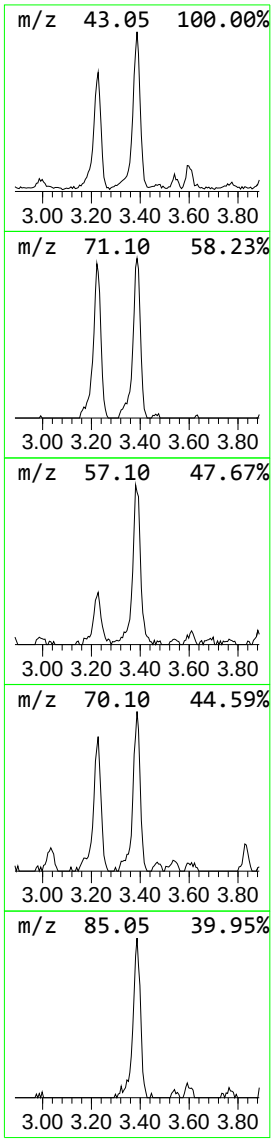
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 2,3,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	3.27 ng	163584	1,4-Dichlorobenzene-d4	6.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	78
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
4	Octane, 4-methyl-	128	C9H20	002216-34-4	64
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130197.D
Acq On : 09 Sep 2022 16:26
Operator : CG\JU
Sample : N4549-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-55

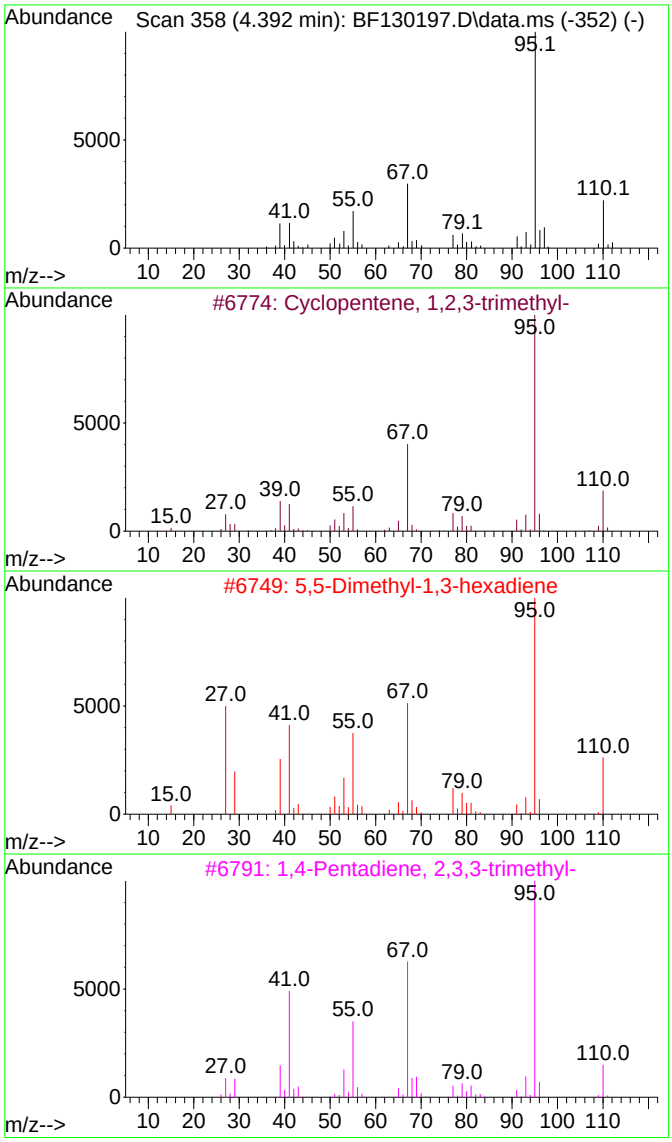
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

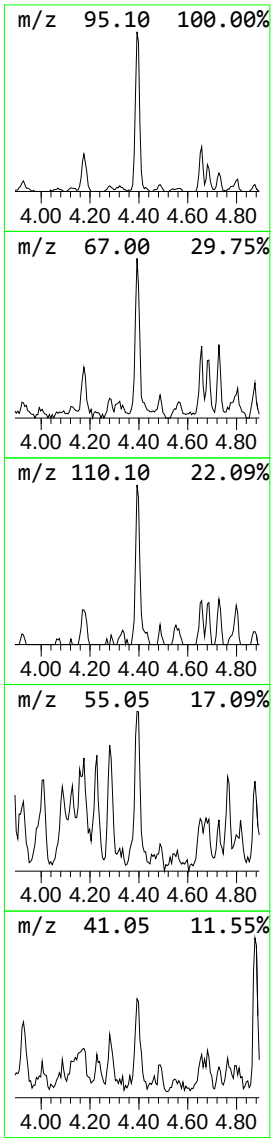
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentene, 1,2,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.392	2.17 ng	108676	1,4-Dichlorobenzene-d4	6.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	90
2	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	87
3	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	83
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	68
5	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130197.D
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Sample : N4549-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-55

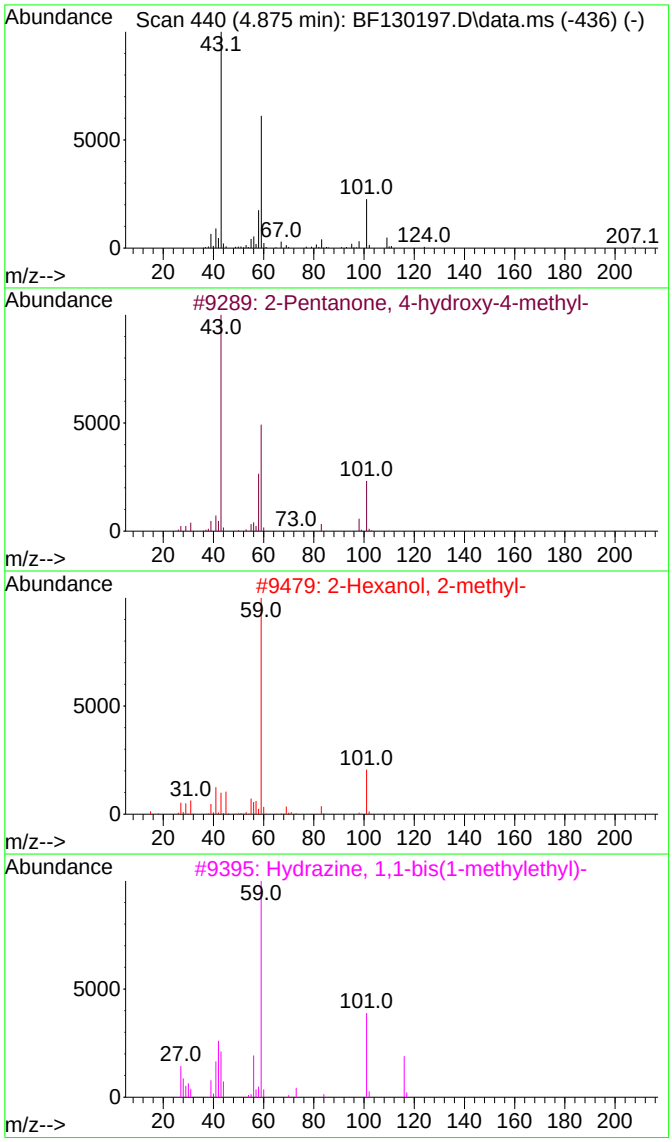
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

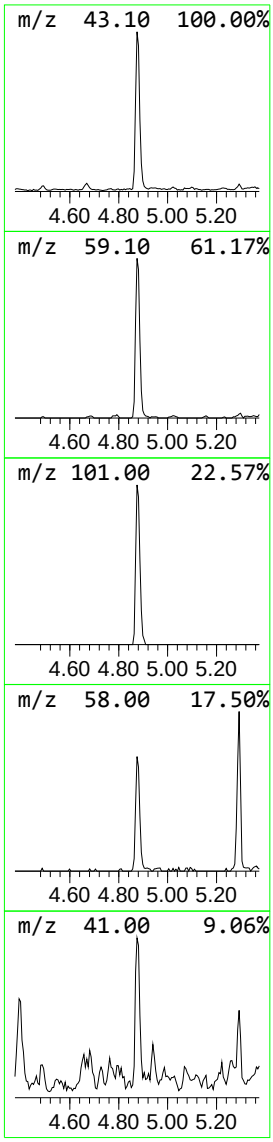
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	3.57 ng	178683	1,4-Dichlorobenzene-d4	6.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	2-Pentanol, 5-methoxy-2-methyl-	132	C7H16O2	055724-04-4	17
5	1-Cyclohexylethanol, methyl ether	142	C9H18O	1000365-12-8	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

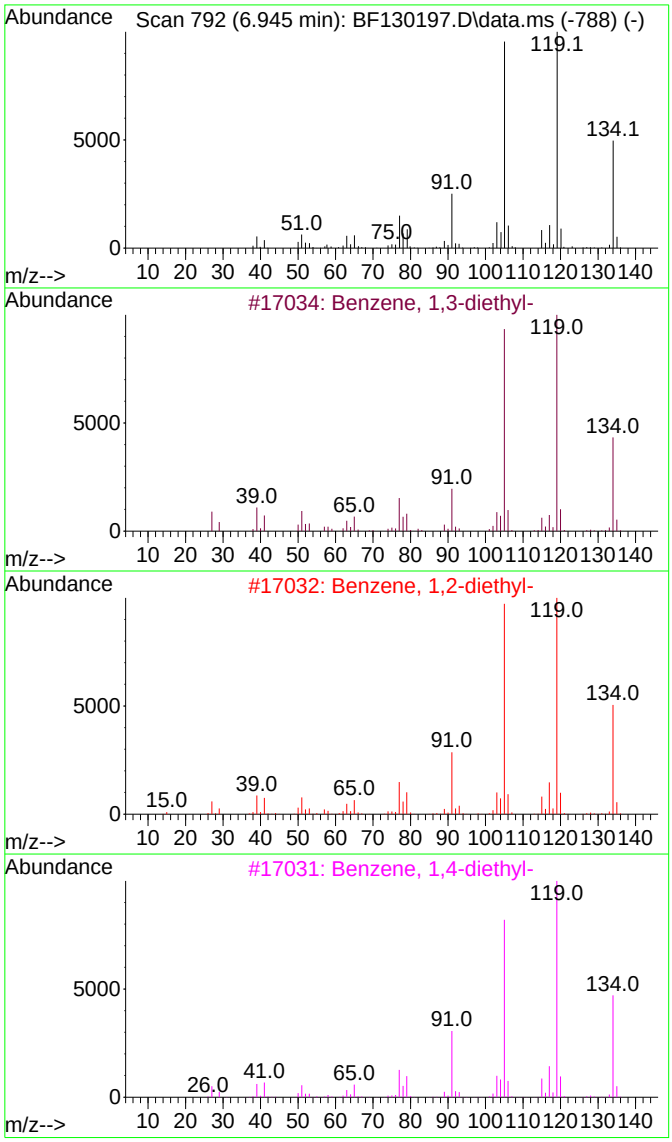
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

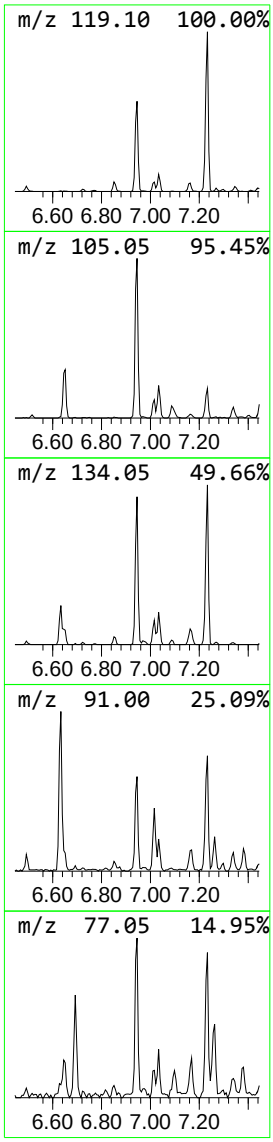
****

Peak Number 5 Benzene, 1,3-diethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.945	4.86 ng	243577	1,4-Dichlorobenzene-d4	6.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	96
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
3	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	95
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90
5	o-Cymene	134	C10H14	000527-84-4	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130197.D
Acq On : 09 Sep 2022 16:26
Operator : CG\JU
Sample : N4549-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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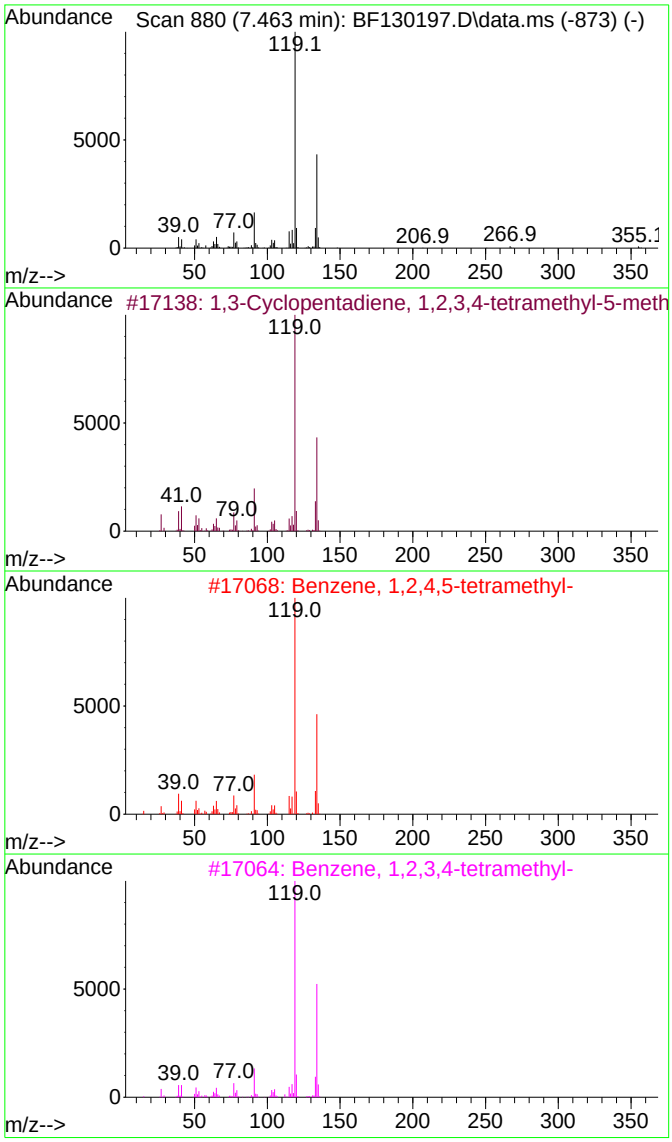
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

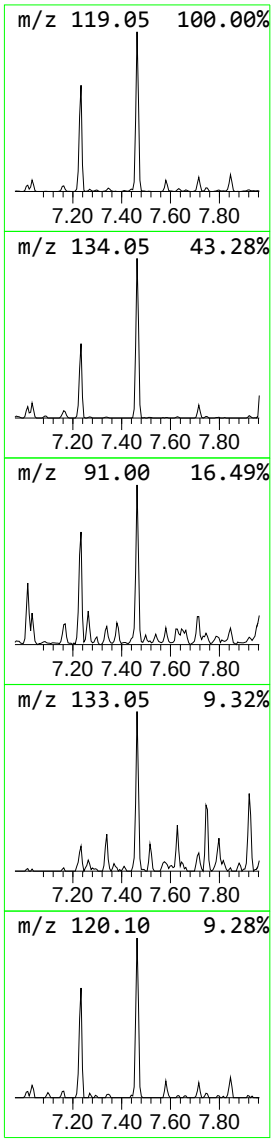
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Cyclopentadiene, 1,2,3,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.463	5.88 ng	433883	Naphthalene-d8	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	97
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
5	o-Cymene	134	C10H14	000527-84-4	93





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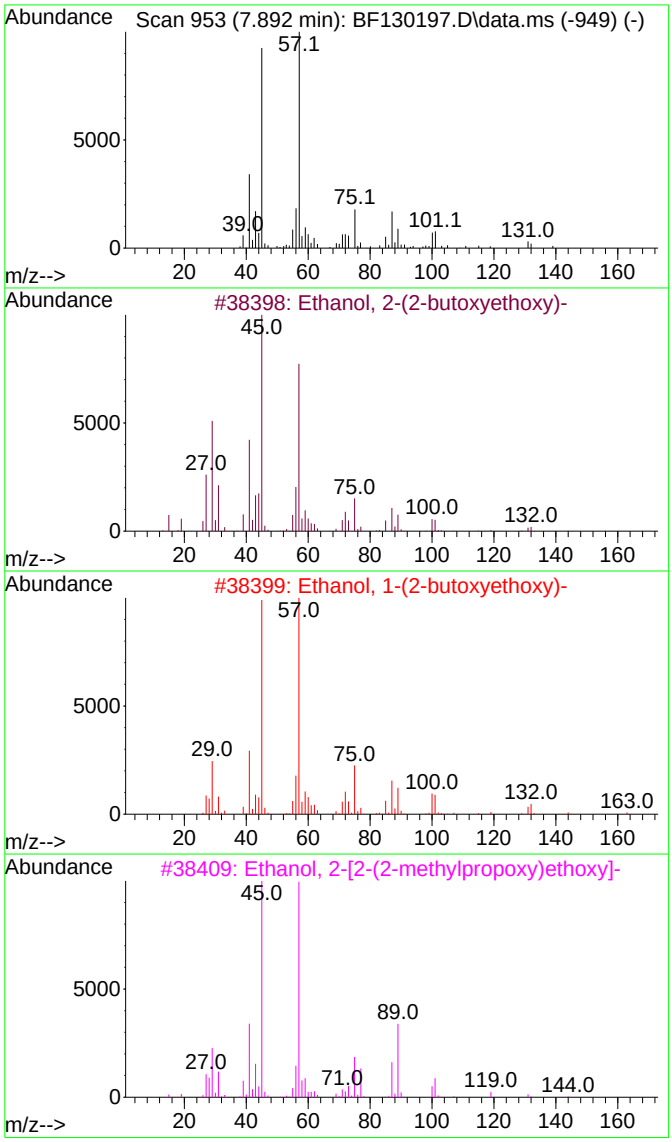
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

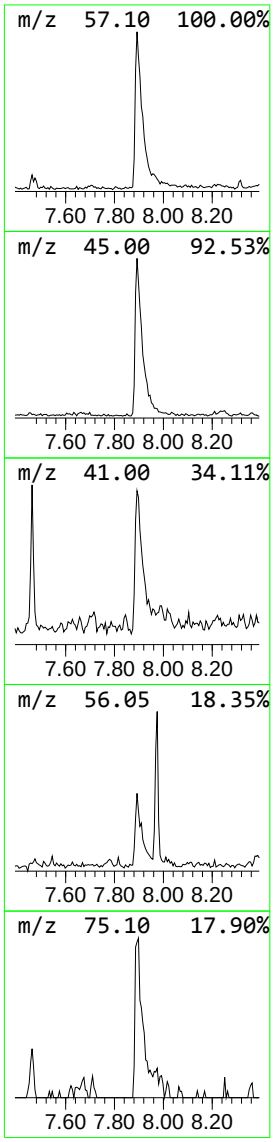
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.892	2.97 ng	219076	Naphthalene-d8	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130197.D
Acq On : 09 Sep 2022 16:26
Operator : CG\JU
Sample : N4549-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

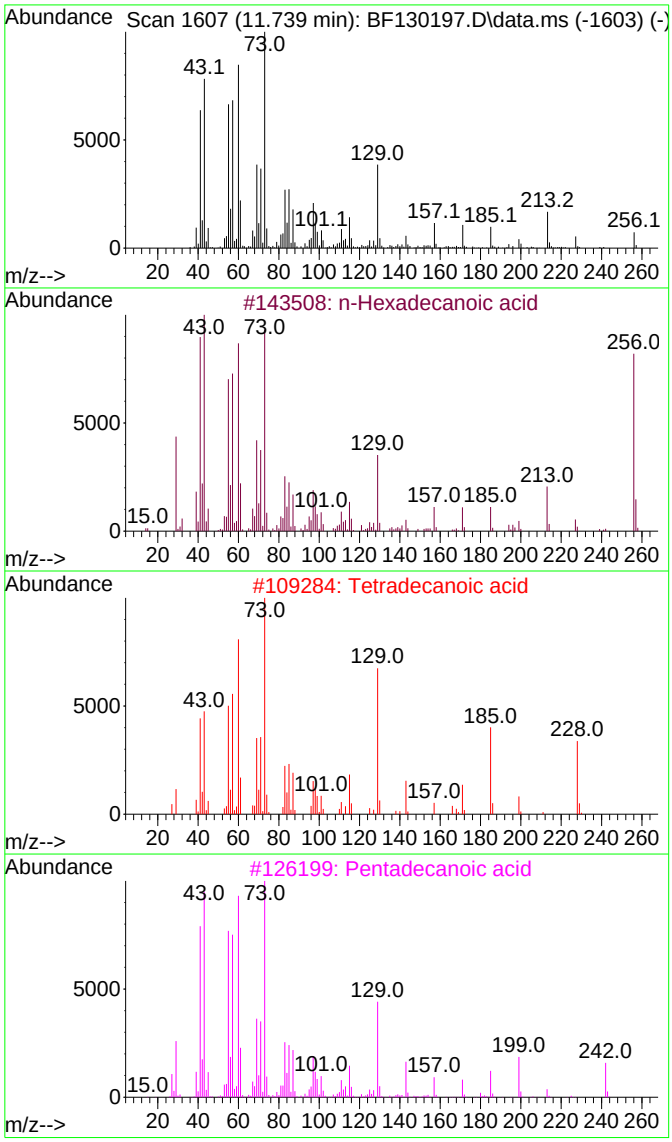
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

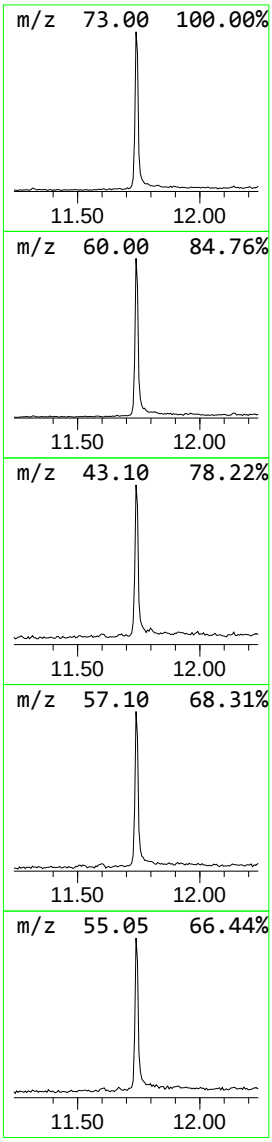
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	10.91 ng	639395	Phenanthrene-d10	11.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Sample : N4549-11
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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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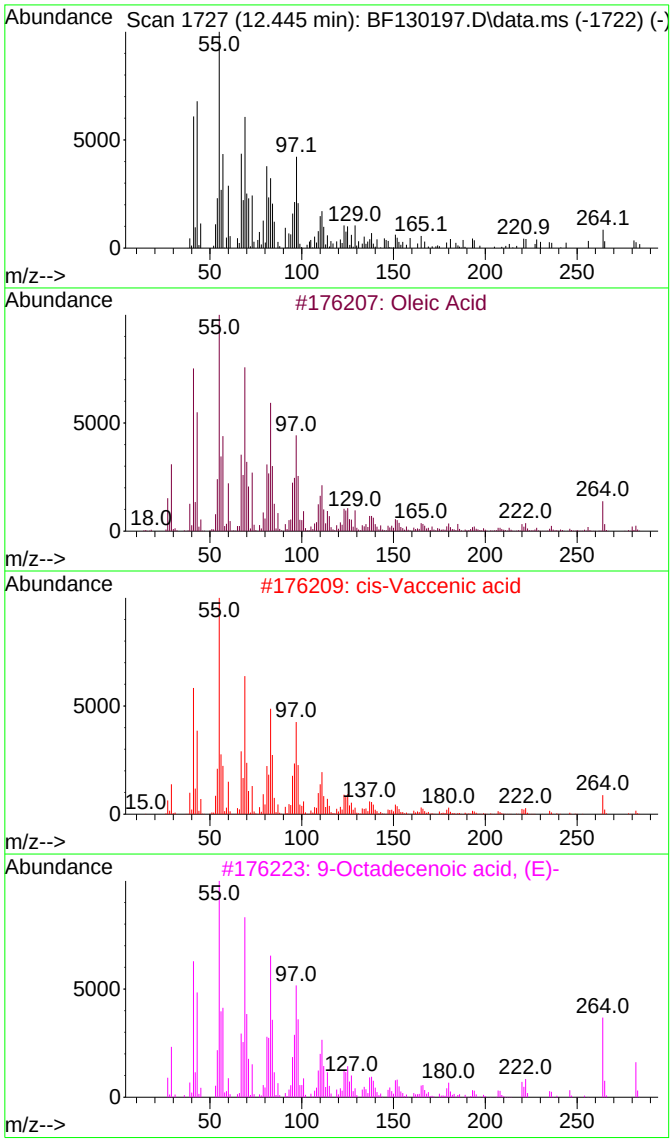
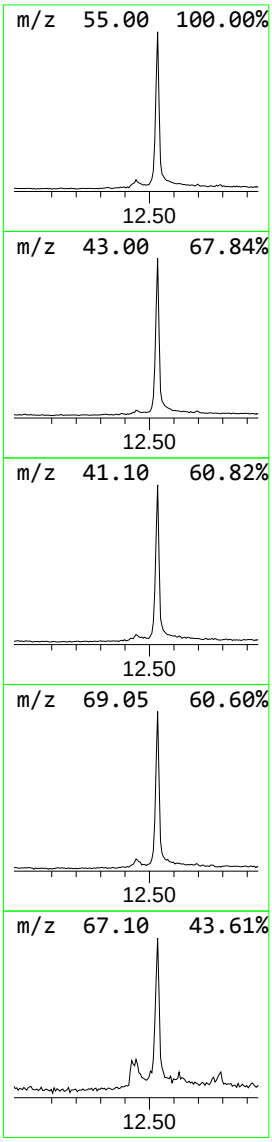
Peak Number 9 Oleic Acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	2.43 ng	142366	Phenanthrene-d10	11.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	97
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	95
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	94
4	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	91
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130197.D
Acq On : 09 Sep 2022 16:26
Operator : CG\JU
Sample : N4549-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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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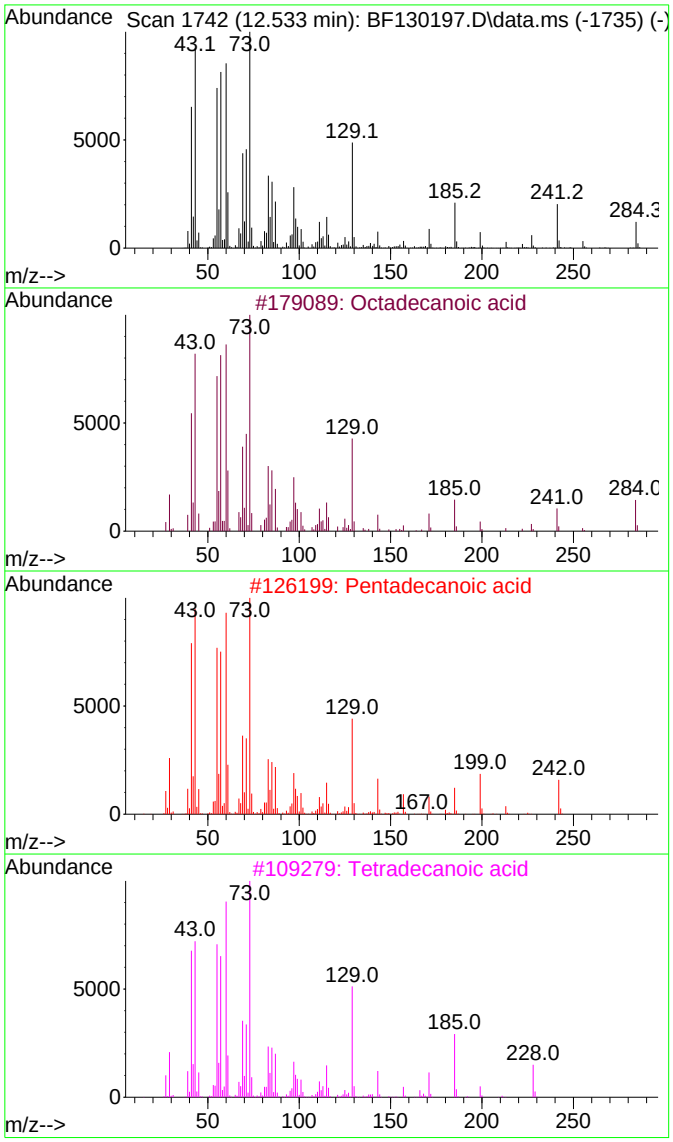
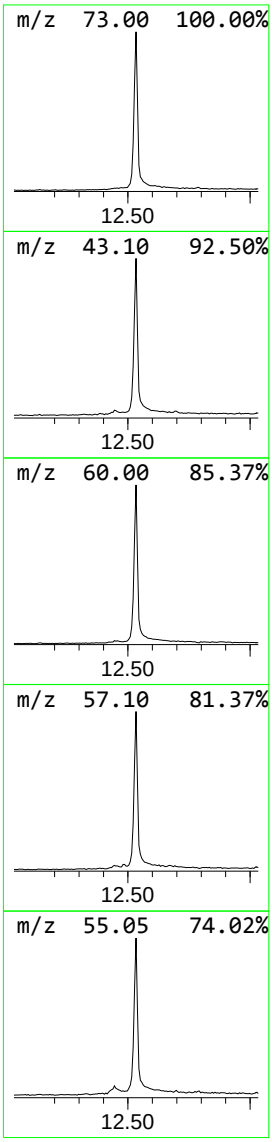
Peak Number 10 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.533	54.31 ng	2277910	Chrysene-d12	13.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130197.D
Acq On : 09 Sep 2022 16:26
Operator : CG\JU
Sample : N4549-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-55

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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
Pentane, 2,3,4-...	3.228	2.5	ng	123098	1	6.692	1001570	20.0
Pentane, 2,3,3-...	3.387	3.3	ng	163584	1	6.692	1001570	20.0
Cyclopentene, 1...	4.392	2.2	ng	108676	1	6.692	1001570	20.0
2-Pentanone, 4-...	4.875	3.6	ng	178683	1	6.692	1001570	20.0
Benzene, 1,3-di...	6.945	4.9	ng	243577	1	6.692	1001570	20.0
1,3-Cyclopentad...	7.463	5.9	ng	433883	2	7.975	1474900	20.0
Ethanol, 2-(2-b...	7.892	3.0	ng	219076	2	7.975	1474900	20.0
n-Hexadecanoic ...	11.739	10.9	ng	639395	4	11.204	1171770	20.0
Oleic Acid	12.445	2.4	ng	142366	4	11.204	1171770	20.0
Octadecanoic acid	12.533	54.3	ng	2277910	5	13.833	838907	20.0