LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134064.D
Acq On : 30 Jun 2023 21:50
Operator : CG\JU
Sample : 03462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-62823

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134064.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	17	rVB	778073	840491	39.07%	5.085%
2	2.228	21	24	28	rVB	28207	35906	1.67%	0.217%
3	5.075	505	508	517	rBV	136069	163436	7.60%	0.989%
4	5.475	572	576	588	rBV	1834449	1745214	81.13%	10.558%
5	6.481	742	747	763	rBV	1913186	1815942	84.41%	10.986%
6	6.845	805	809	821	rBV	733518	617428	28.70%	3.735%
7	7.404	900	904	915	rBV	1323536	1185588	55.11%	7.173%
8	8.122	1023	1026	1035	rVB	941541	774808	36.02%	4.688%
9	9.198	1206	1209	1213	rBV	2349394	2151249	100.00%	13.015%
10	9.810	1310	1313	1316	rBV	35433	26866	1.25%	0.163%
11	9.880	1322	1325	1329	rBV	1029383	864970	40.21%	5.233%
12	10.310	1396	1398	1401	rVB	45485	37662	1.75%	0.228%
13	10.533	1431	1436	1441	rBV2	27041	40530	1.88%	0.245%
14	10.598	1443	1447	1450	rBV	419093	337152	15.67%	2.040%
15	10.674	1456	1460	1467	rBV	1261968	1076404	50.04%	6.512%
16	10.786	1476	1479	1480	rBV	51637	40870	1.90%	0.247%
17	10.910	1497	1500	1509	rVB2	81992	102067	4.74%	0.617%
18	11.239	1553	1556	1558	rBV	54803	46923	2.18%	0.284%
19	11.269	1558	1561	1566	rVB2	53325	65962	3.07%	0.399%
20	11.374	1576	1579	1583	rBV	928908	806586	37.49%	4.880%
21	11.480	1595	1597	1600	rBV2	34871	28646	1.33%	0.173%
22	11.621	1617	1621	1624	rBV4	19245	23231	1.08%	0.141%
23	11.669	1626	1629	1634	rVB	47341	41963	1.95%	0.254%
24	11.769	1643	1646	1652	rVB	63507	63662	2.96%	0.385%
25	11.904	1666	1669	1674	rBV	101533	114791	5.34%	0.694%
26	12.074	1695	1698	1704	rVB2	48299	51185	2.38%	0.310%
27	12.463	1760	1764	1766	rBV2	210064	231408	10.76%	1.400%
28	12.480	1766	1767	1773	rVB2	186013	131494	6.11%	0.796%
29	12.568	1779	1782	1785	rVB2	47402	39375	1.83%	0.238%
30	12.698	1801	1804	1809	rVB7	21109	26721	1.24%	0.162%
31	12.845	1827	1829	1831	rVB2	41888	29537	1.37%	0.179%
32	12.974	1846	1851	1854	rBV	1524068	1495183	69.50%	9.046%
33	13.204	1887	1890	1895	rBV	49358	43443	2.02%	0.263%
34	13.551	1946	1949	1951	rVB	46282	42585	1.98%	0.258%
35	13.880	2002	2005	2007	rBV	56853	54765	2.55%	0.331%
36	13.910	2007	2010	2017	rVB3	49840	90822	4.22%	0.549%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134064.D
Acq On : 30 Jun 2023 21:50
Operator : CG\JU
Sample : 03462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-62823

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.033	2027	2031	2038	rBV	570707	537013	24.96%	3.249%
38	14.198	2056	2059	2064	rVB	66790	60722	2.82%	0.367%
39	14.510	2109	2112	2115	rBV	55171	50187	2.33%	0.304%
40	14.821	2163	2165	2168	rVB	42119	38204	1.78%	0.231%
41	15.174	2222	2225	2229	rVB2	42767	46442	2.16%	0.281%
42	15.539	2283	2287	2291	rBV	415943	511708	23.79%	3.096%

Sum of corrected areas: 16529141

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Instrument :
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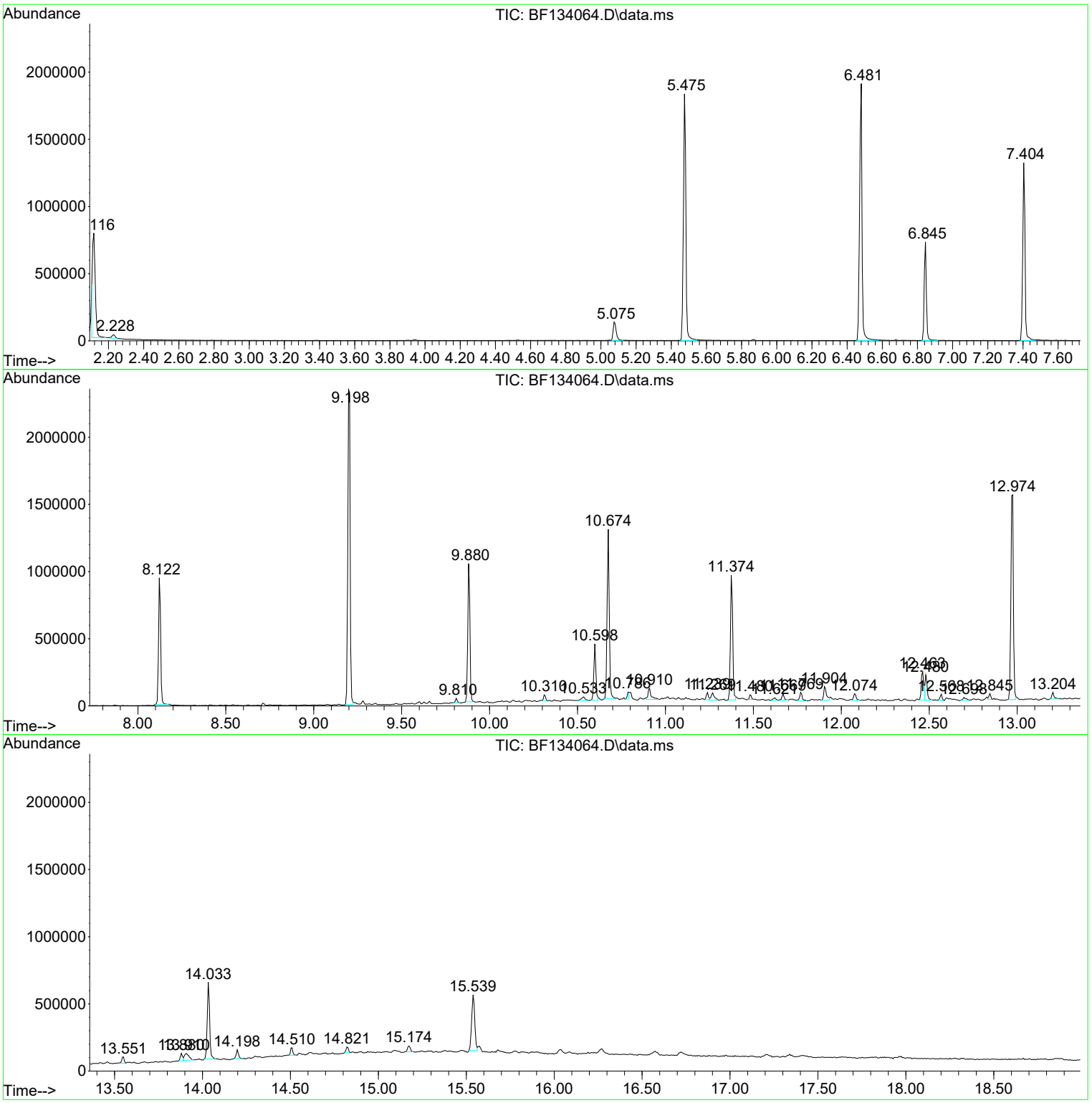
ClientSampleId :
SU-02-62823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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\BF063023\
Data File : BF134064.D
Acq On : 30 Jun 2023 21:50
Operator : CG\JU
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

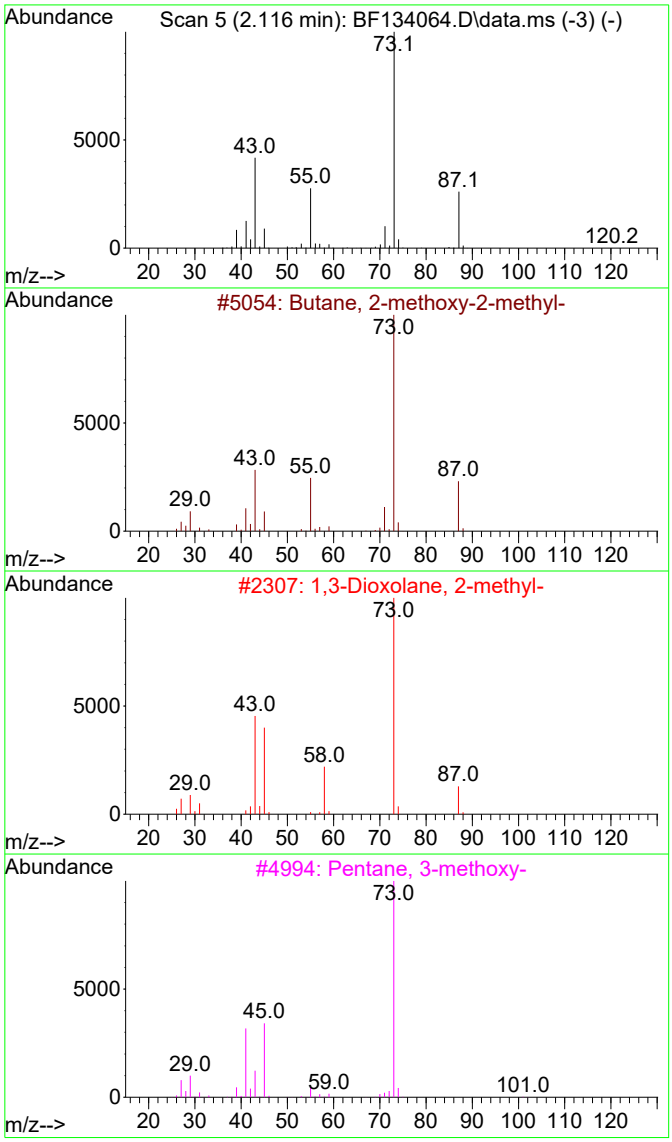
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

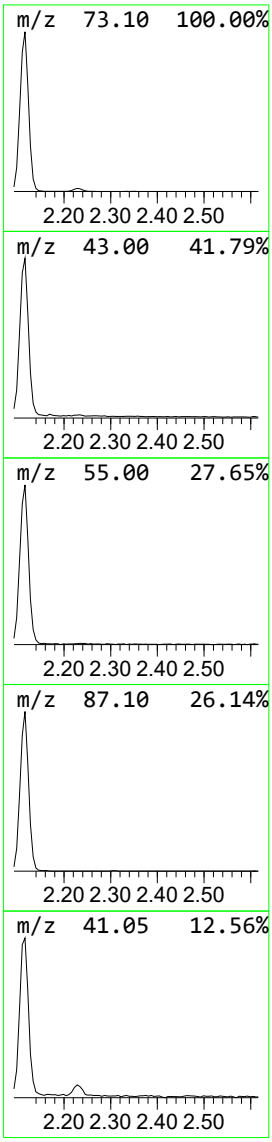
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	27.23 ng	840491	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Operator : CG\JU
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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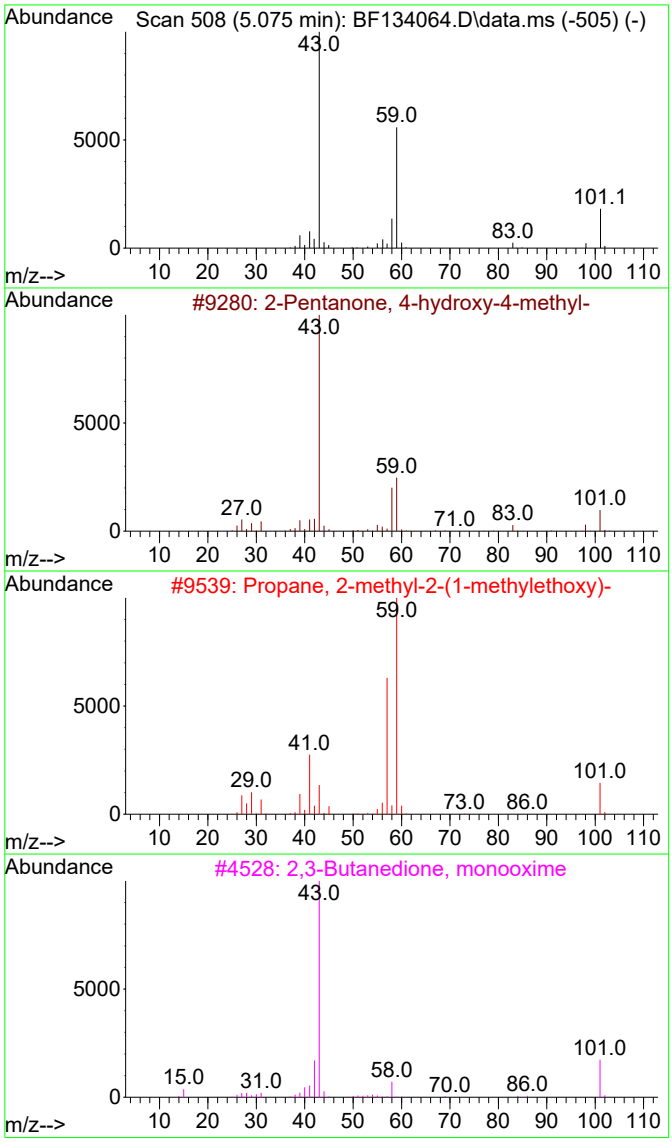
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

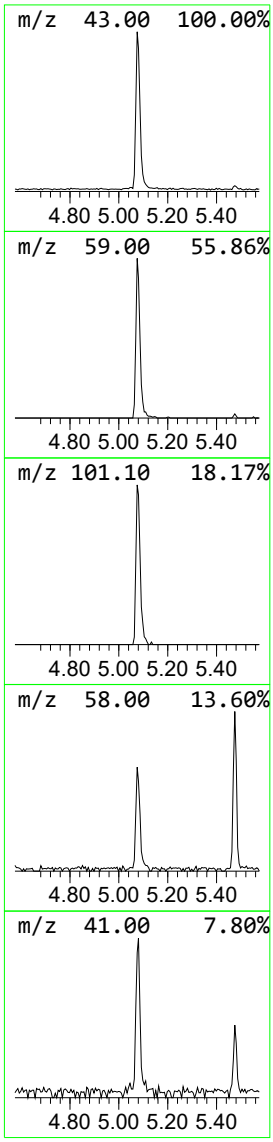
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	5.29 ng	163436	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Data File : BF134064.D
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Operator : CG\JU
Sample : 03462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-62823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

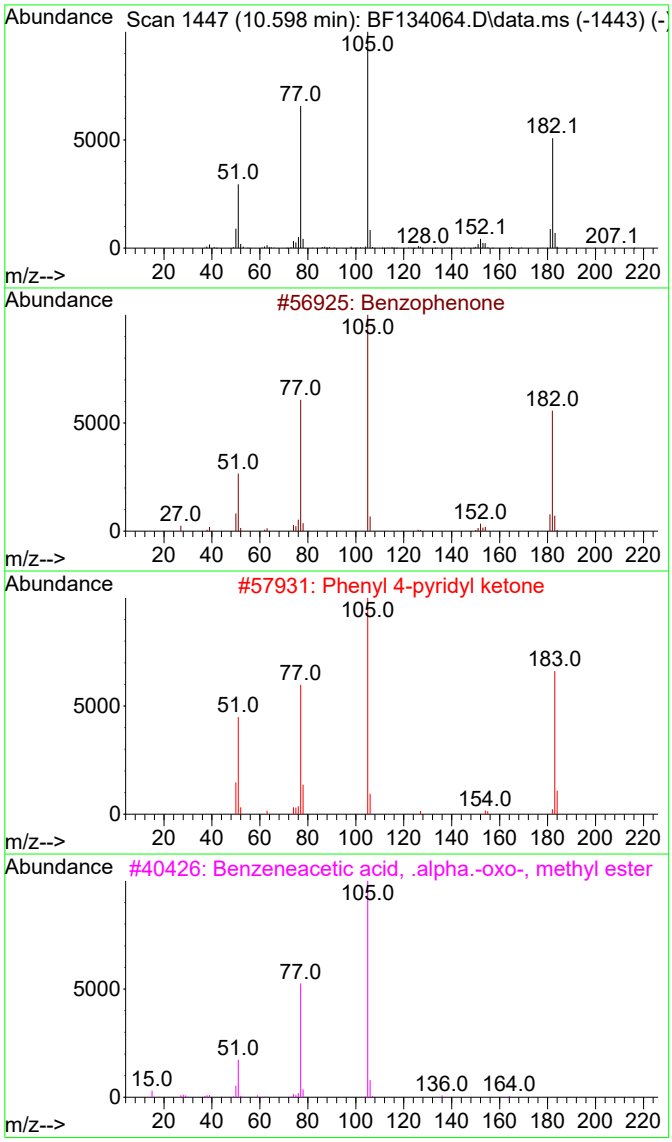
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

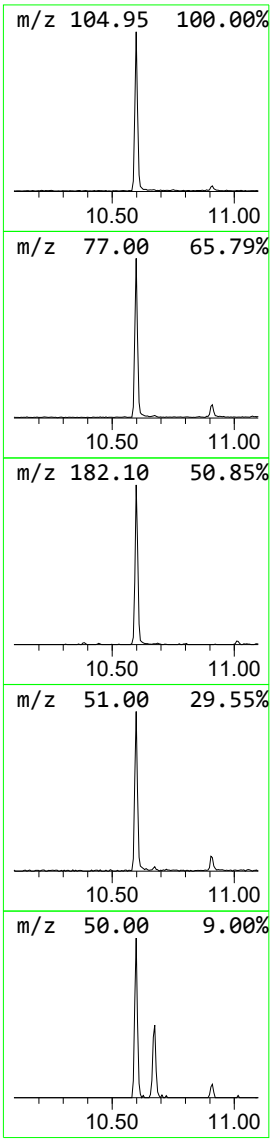
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	7.80 ng	337152	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
4	Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
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Acq On : 30 Jun 2023 21:50
Operator : CG\JU
Sample : 03462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-62823

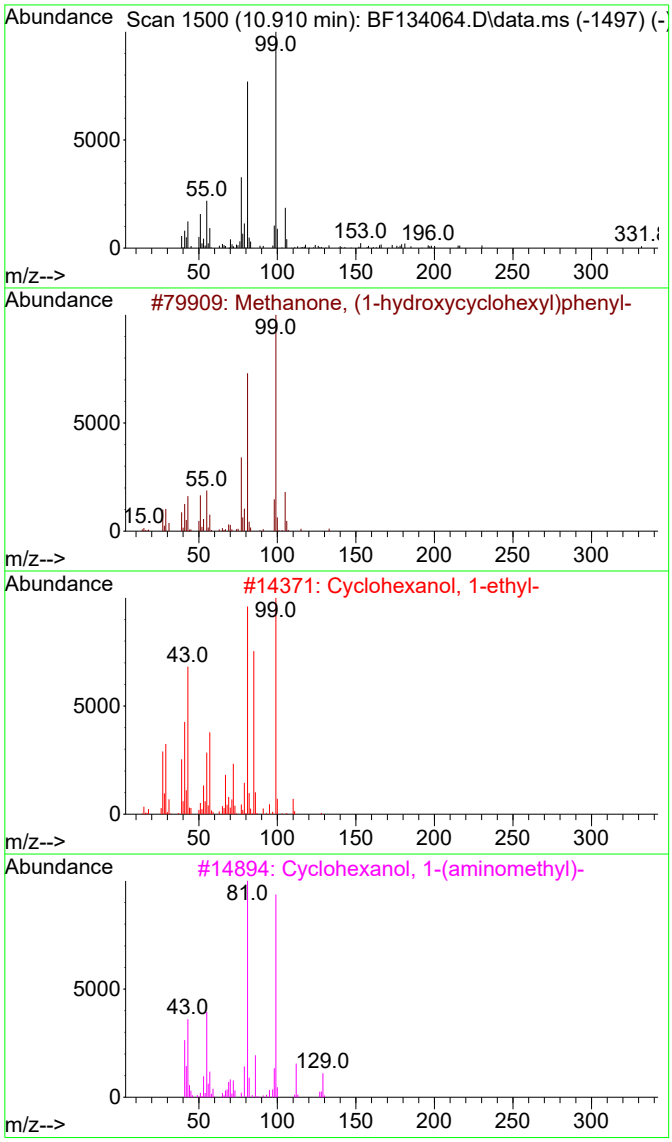
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

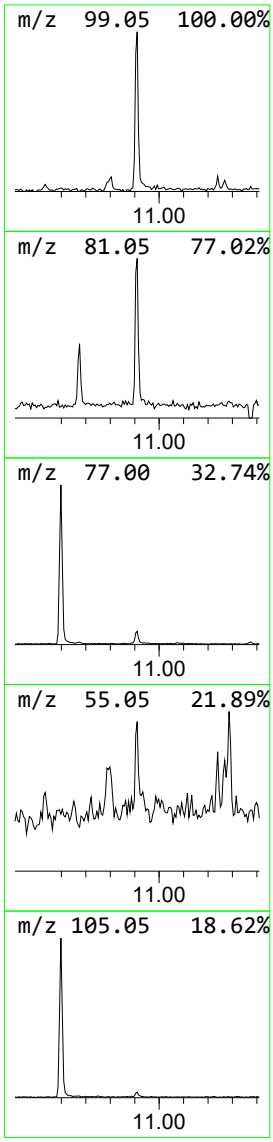
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Methanone, (1-hydroxycycloh... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.910	2.53 ng	102067	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2	Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	59
3	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	50
4	1-(Prop-2-yn-1-yl)cyclohexyl car...	181	C10H15NO2	000358-52-1	39
5	Cyclohexane, 1,2-dichloro-	152	C6H10Cl2	001121-21-7	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134064.D
Acq On : 30 Jun 2023 21:50
Operator : CG\JU
Sample : 03462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-62823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

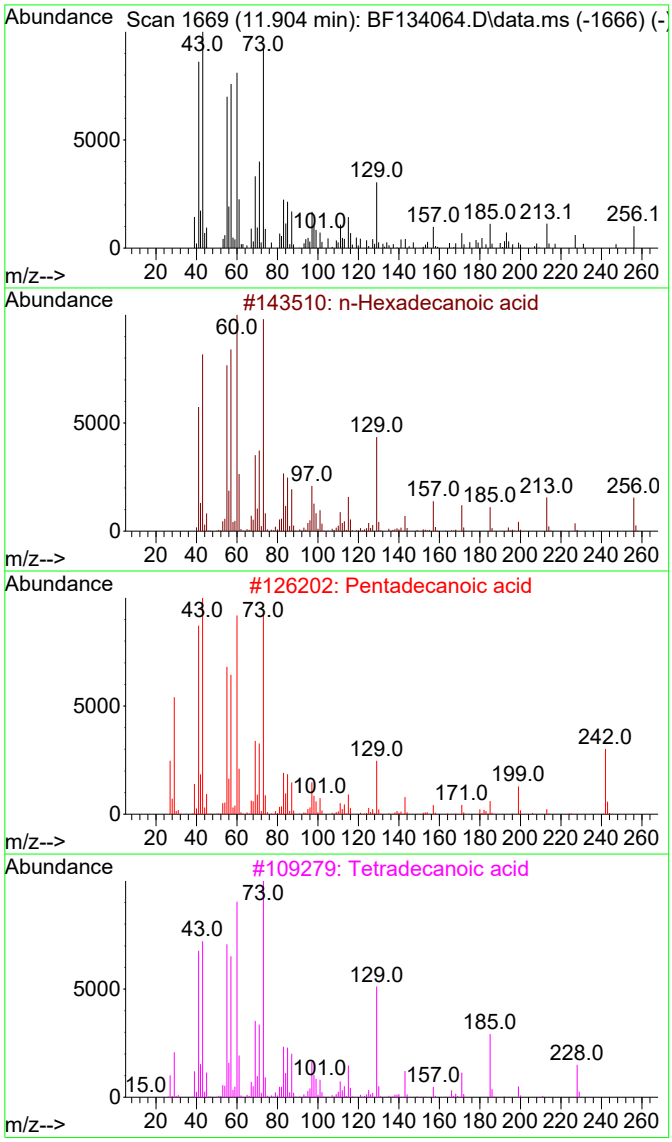
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

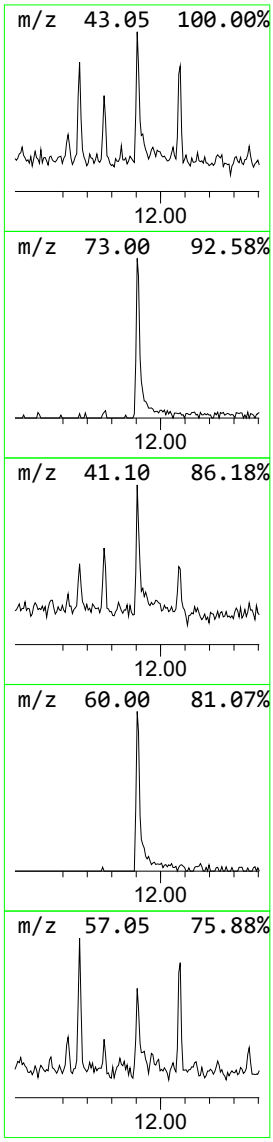
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	2.85 ng	114791	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43





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Instrument :
BNA_F
ClientSampleId :
SU-02-62823

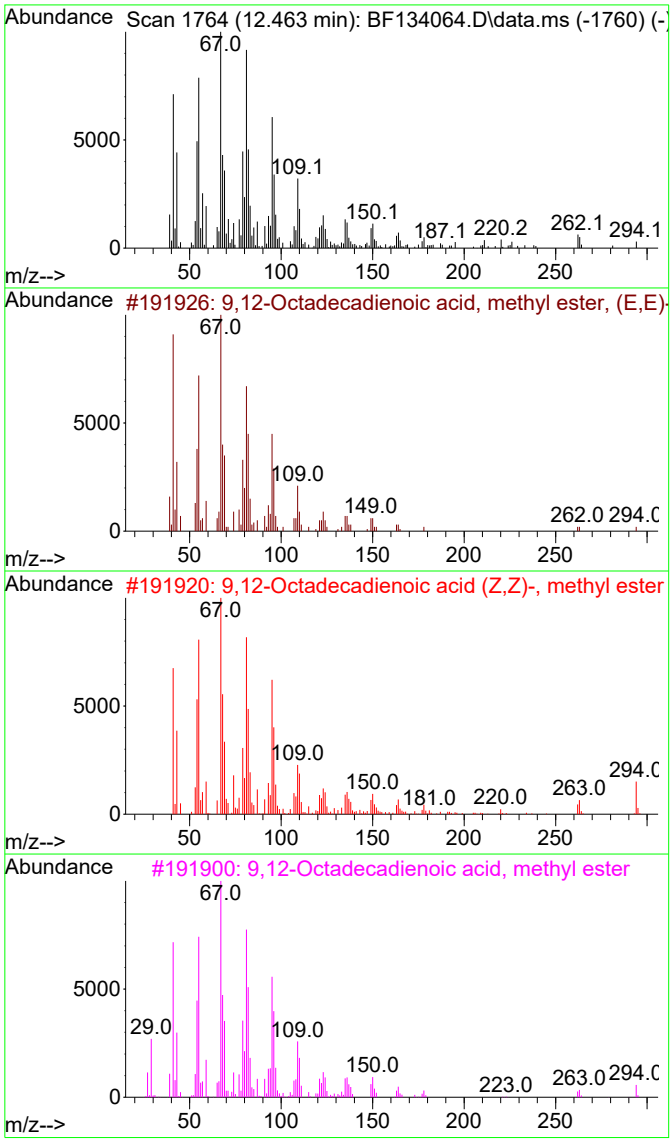
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

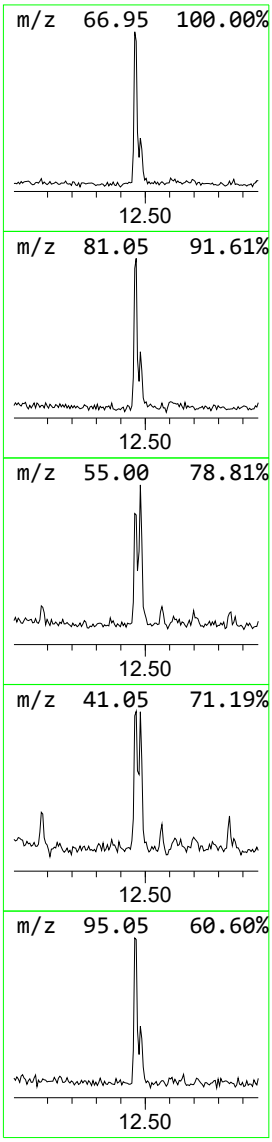
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	5.74 ng	231408	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	94
4	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	93
5	Linoelaidic acid	280	C18H32O2	000506-21-8	90





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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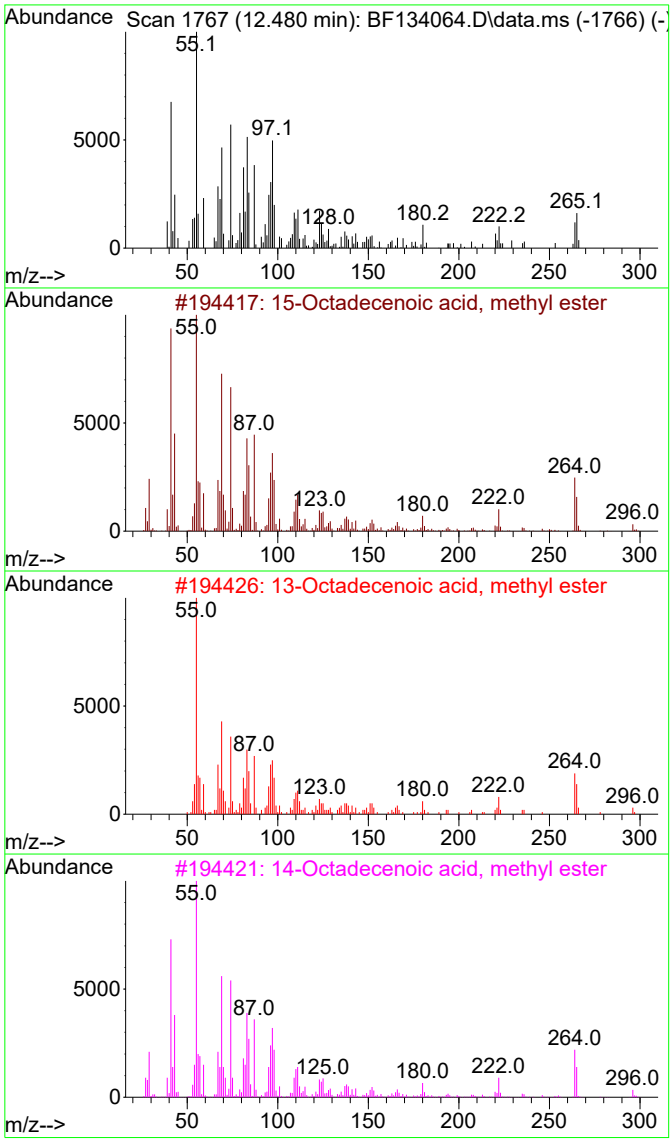
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

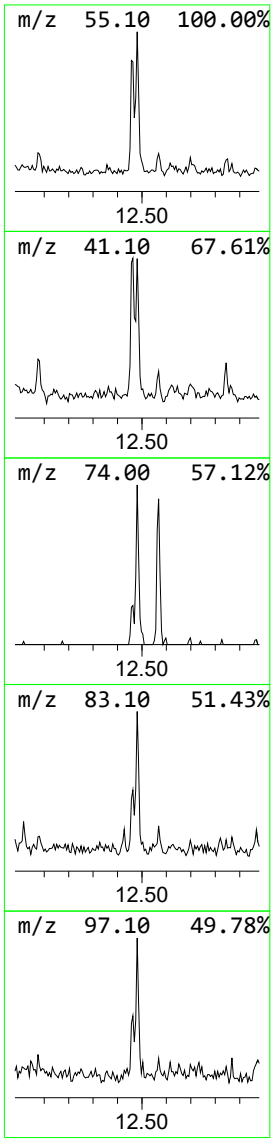
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 15-Octadecenoic acid, methy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.480	3.26 ng	131494	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	74
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	74
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	72
4	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	68
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	64





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Data File : BF134064.D
Acq On : 30 Jun 2023 21:50
Operator : CG\JU
Sample : 03462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-62823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

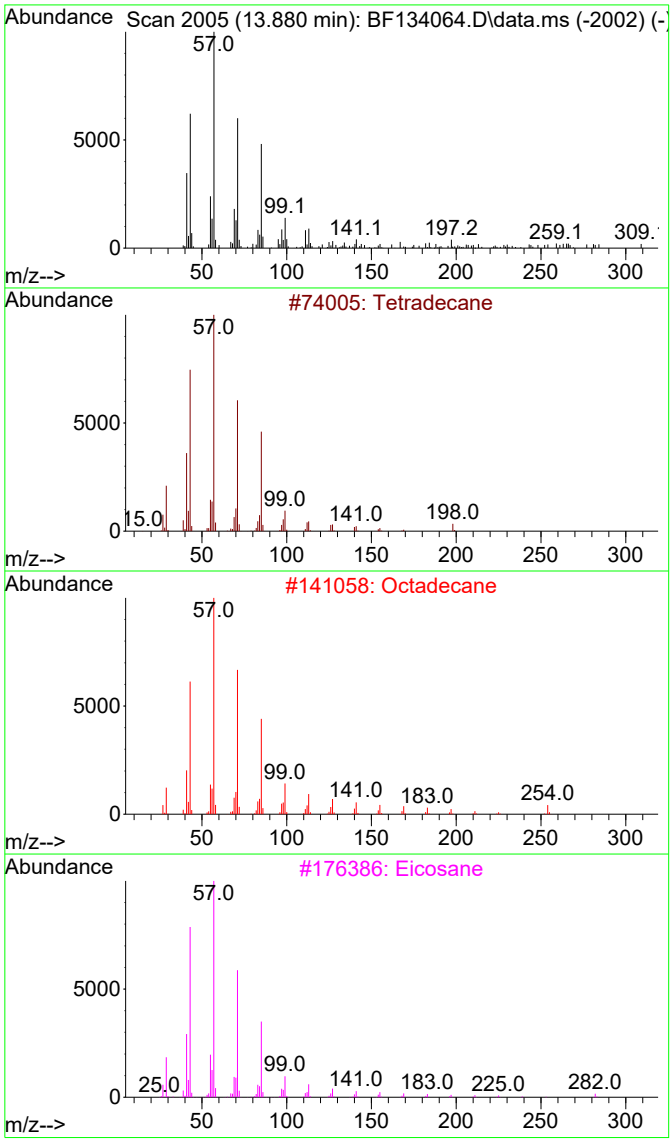
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

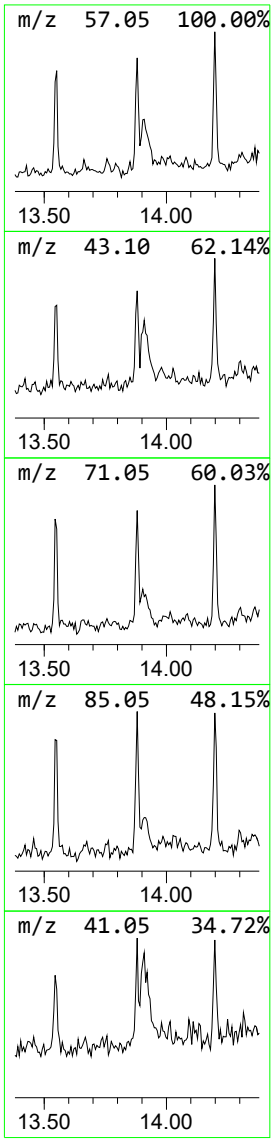
****

Peak Number 8 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	2.04 ng	54765	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	87
2	Octadecane	254	C18H38	000593-45-3	87
3	Eicosane	282	C20H42	000112-95-8	86
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	83
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	81





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-62823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

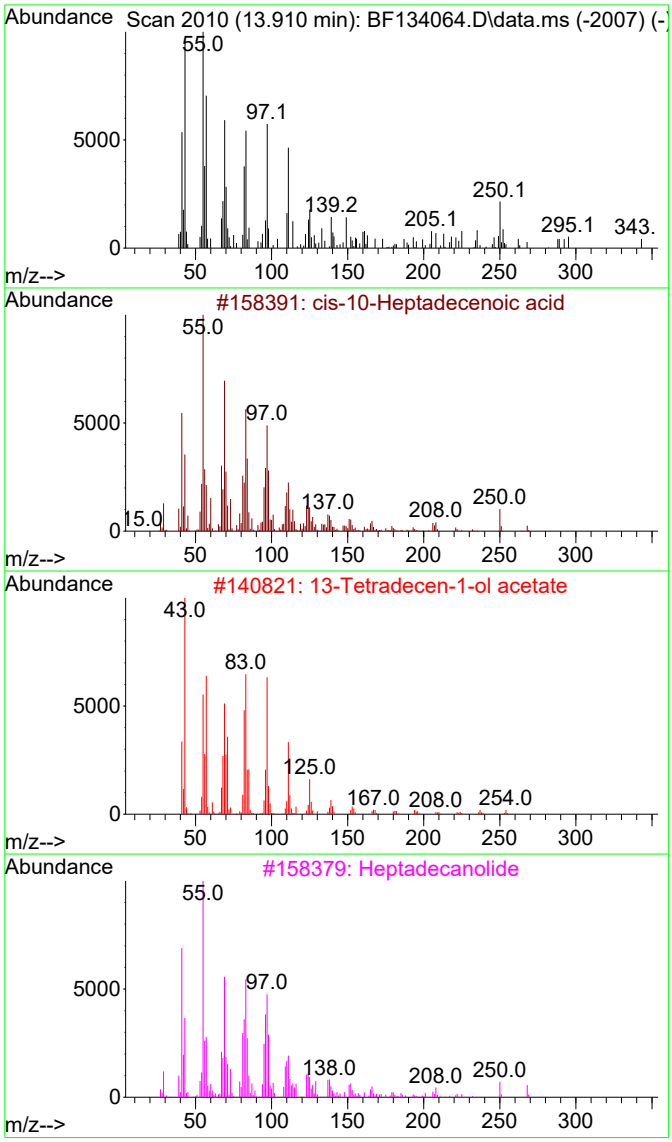
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

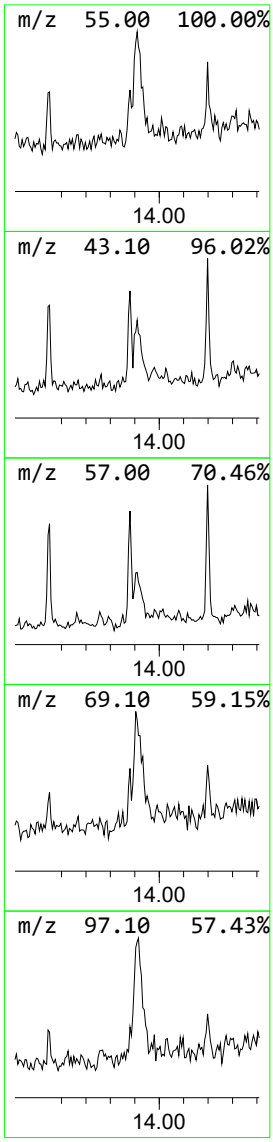
****

Peak Number 9 cis-10-Heptadecenoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	3.38 ng	90822	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-10-Heptadecenoic acid	268	C17H32O2	029743-97-3	52
2	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	49
3	Heptadecanolide	268	C17H32O2	005637-97-8	47
4	1-Docosene	308	C22H44	001599-67-3	46
5	1-Hexacosene	364	C26H52	018835-33-1	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134064.D
Acq On : 30 Jun 2023 21:50
Operator : CG\JU
Sample : 03462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-62823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

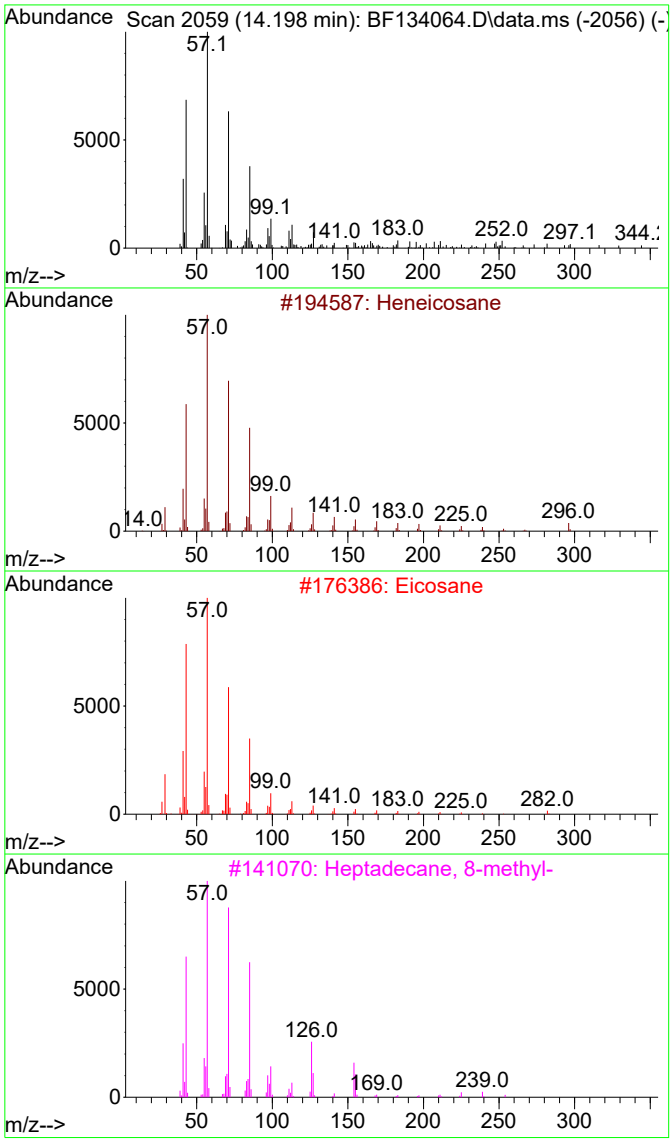
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

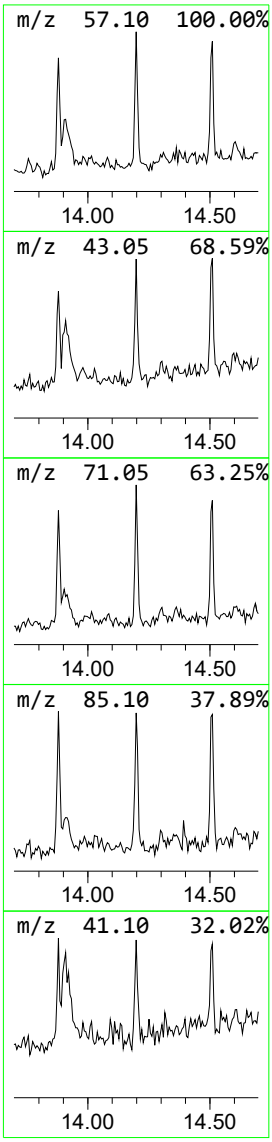
****

Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	2.26 ng	60722	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Eicosane	282	C20H42	000112-95-8	90
3	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	89
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptacosane	380	C27H56	000593-49-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134064.D
Acq On : 30 Jun 2023 21:50
Operator : CG\JU
Sample : 03462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-62823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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...	2.116	27.2	ng	840491	1	6.845	617428	20.0
2-Pentanone, 4-...	5.075	5.3	ng	163436	1	6.845	617428	20.0
Benzophenone	10.598	7.8	ng	337152	3	9.880	864970	20.0
Methanone, (1-h...	10.910	2.5	ng	102067	4	11.374	806586	20.0
n-Hexadecanoic ...	11.904	2.9	ng	114791	4	11.374	806586	20.0
9,12-Octadecadi...	12.463	5.7	ng	231408	4	11.374	806586	20.0
15-Octadecenoic...	12.480	3.3	ng	131494	4	11.374	806586	20.0
Tetradecane	13.880	2.0	ng	54765	5	14.033	537013	20.0
cis-10-Heptadec...	13.910	3.4	ng	90822	5	14.033	537013	20.0
Heneicosane	14.198	2.3	ng	60722	5	14.033	537013	20.0