LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131581.D
Acq On : 09 Dec 2022 22:57
Operator : CG\JU
Sample : N5943-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RM-301

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: BF131581.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	10	17	23	rBV	445706	542923	32.85%	4.374%
2	2.299	31	36	42	rBV	24106	33899	2.05%	0.273%
3	3.428	224	228	236	rBV	13443	25362	1.53%	0.204%
4	4.498	406	410	416	rBV	32059	36357	2.20%	0.293%
5	5.128	511	517	527	rVB	517137	628292	38.02%	5.061%
6	5.528	580	585	588	rBV	1545116	1339896	81.08%	10.794%
7	5.740	618	621	626	rBV	33359	29211	1.77%	0.235%
8	5.916	648	651	655	rBV	57681	48136	2.91%	0.388%
9	6.539	752	757	760	rBV	1485866	1448202	87.63%	11.667%
10	6.910	816	820	823	rBV	477079	379237	22.95%	3.055%
11	7.475	911	916	919	rBV	977641	942465	57.03%	7.592%
12	8.198	1035	1039	1042	rBV	543039	435885	26.38%	3.511%
13	8.222	1042	1043	1046	rVB	42183	20866	1.26%	0.168%
14	9.280	1217	1223	1226	rBV	2098037	1652596	100.00%	13.313%
15	9.963	1335	1339	1342	rVB	538871	436206	26.40%	3.514%
16	10.380	1408	1410	1413	rVB2	24199	22540	1.36%	0.182%
17	10.674	1454	1460	1462	rBV2	18380	22653	1.37%	0.182%
18	10.751	1469	1473	1476	rBV	804489	620901	37.57%	5.002%
19	10.869	1486	1493	1497	rVB4	27442	42488	2.57%	0.342%
20	10.951	1501	1507	1512	rBV7	11154	22031	1.33%	0.177%
21	11.310	1564	1568	1570	rBV3	26440	27392	1.66%	0.221%
22	11.339	1570	1573	1578	rVB3	20086	30101	1.82%	0.242%
23	11.457	1589	1593	1595	rBV	416633	390447	23.63%	3.145%
24	11.474	1595	1596	1600	rVV	127681	105603	6.39%	0.851%
25	11.527	1601	1605	1608	rVB	41793	40538	2.45%	0.327%
26	11.616	1617	1620	1625	rBV4	14705	21388	1.29%	0.172%
27	11.686	1629	1632	1637	rBV3	20719	25405	1.54%	0.205%
28	11.839	1655	1658	1661	rBV	57317	43897	2.66%	0.354%
29	11.957	1674	1678	1679	rBV	26182	24878	1.51%	0.200%
30	11.980	1679	1682	1686	rVB2	37253	50559	3.06%	0.407%
31	12.069	1694	1697	1699	rBV2	33639	35306	2.14%	0.284%
32	12.533	1773	1776	1778	rBV2	62629	69181	4.19%	0.557%
33	12.551	1778	1779	1784	rVB2	72728	49766	3.01%	0.401%
34	12.668	1796	1799	1803	rBV	184349	170110	10.29%	1.370%
35	12.904	1833	1839	1844	rBV	201344	219589	13.29%	1.769%
36	13.045	1859	1863	1870	rVB	1321804	1160651	70.23%	9.350%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131581.D
Acq On : 09 Dec 2022 22:57
Operator : CG\JU
Sample : N5943-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RM-301

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

37	13.116	1872	1875	1880	rBV5	18513	34013	2.06%	0.274%
38	13.227	1892	1894	1898	rVB2	34882	33206	2.01%	0.268%
39	13.268	1899	1901	1904	rBV3	25023	26865	1.63%	0.216%
40	13.615	1958	1960	1962	rBV2	26535	22812	1.38%	0.184%
41	14.104	2039	2043	2046	rBV2	356020	392215	23.73%	3.160%
42	14.133	2046	2048	2055	rVB	75038	73250	4.43%	0.590%
43	14.204	2055	2060	2064	rBV	283716	312558	18.91%	2.518%
44	15.627	2298	2302	2310	rVB	199385	323421	19.57%	2.605%

Sum of corrected areas: 12413297

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Instrument :
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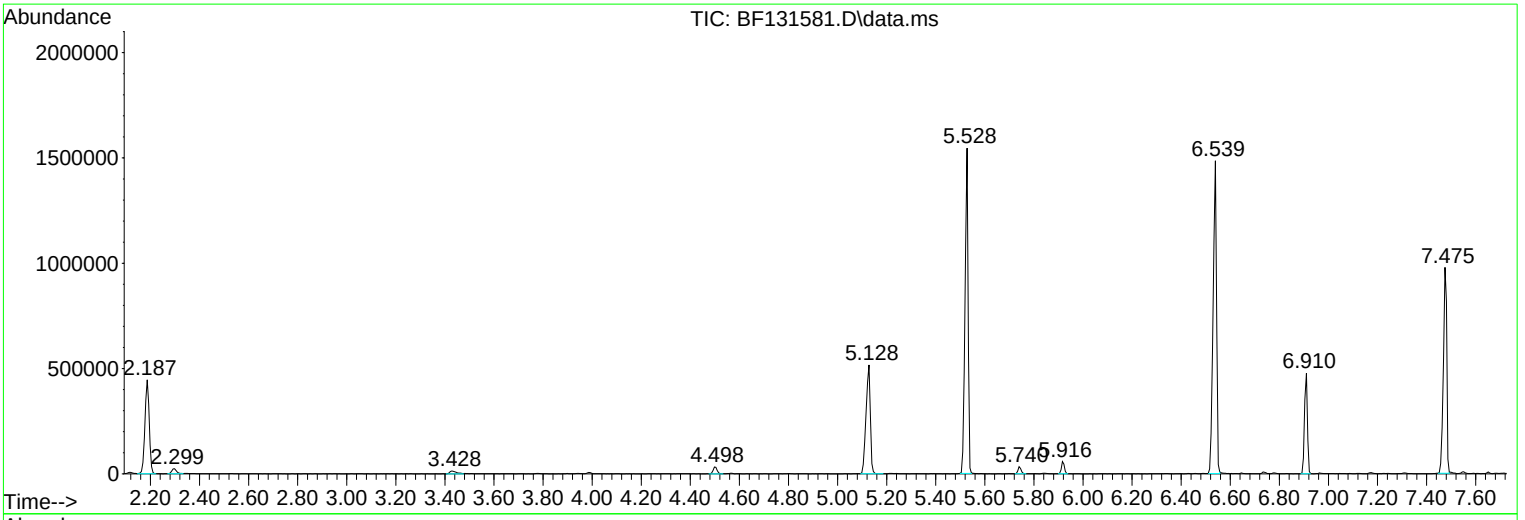
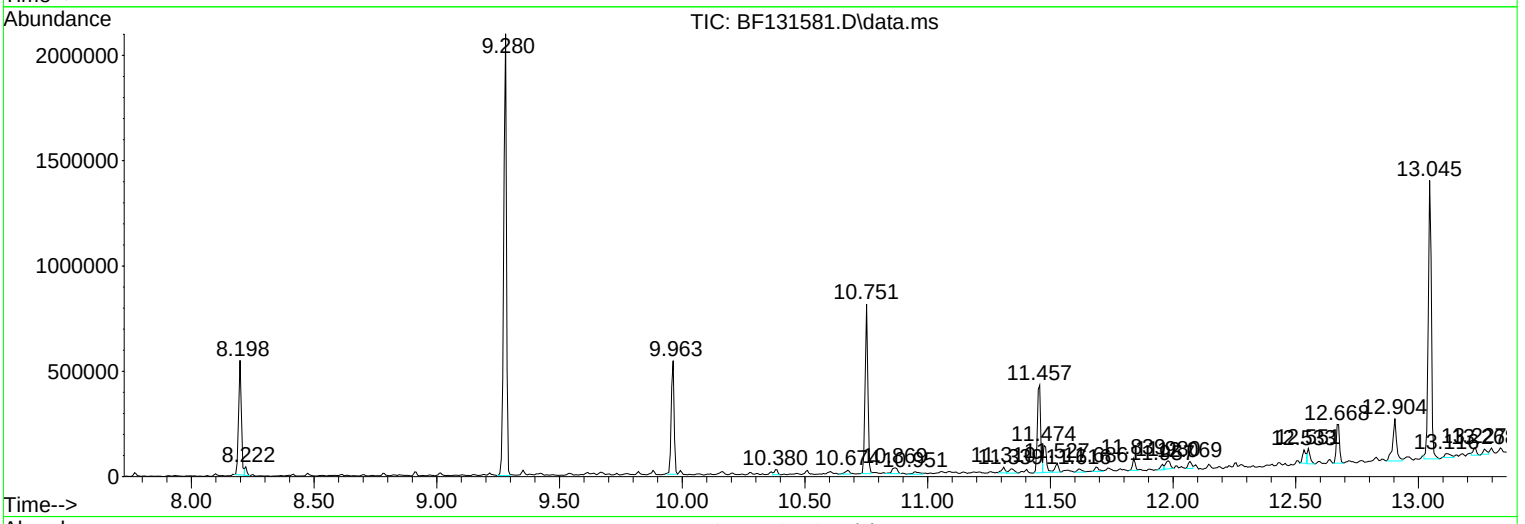
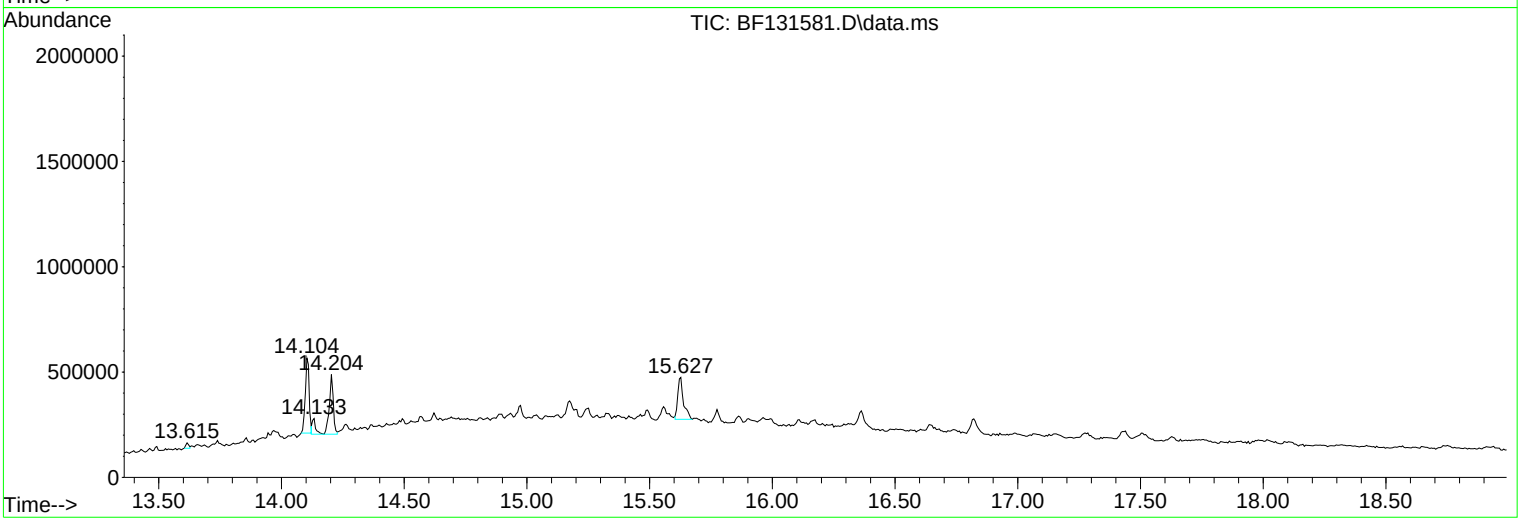
ClientSampleId :
RM-301

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\BF120922\
Data File : BF131581.D
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Sample : N5943-01
Misc :
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Instrument :
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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

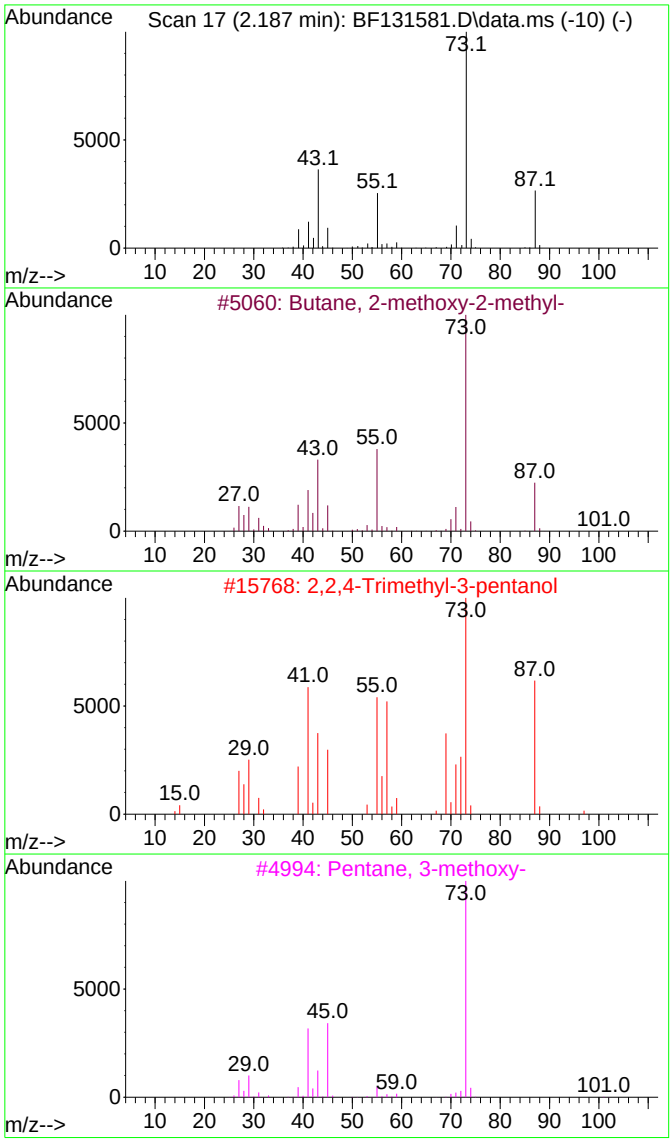
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

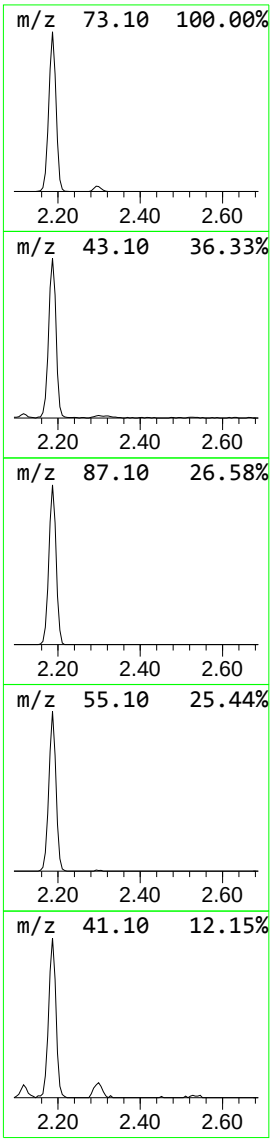
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	28.63 ng	542923	1,4-Dichlorobenzene-d4	6.910

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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RM-301

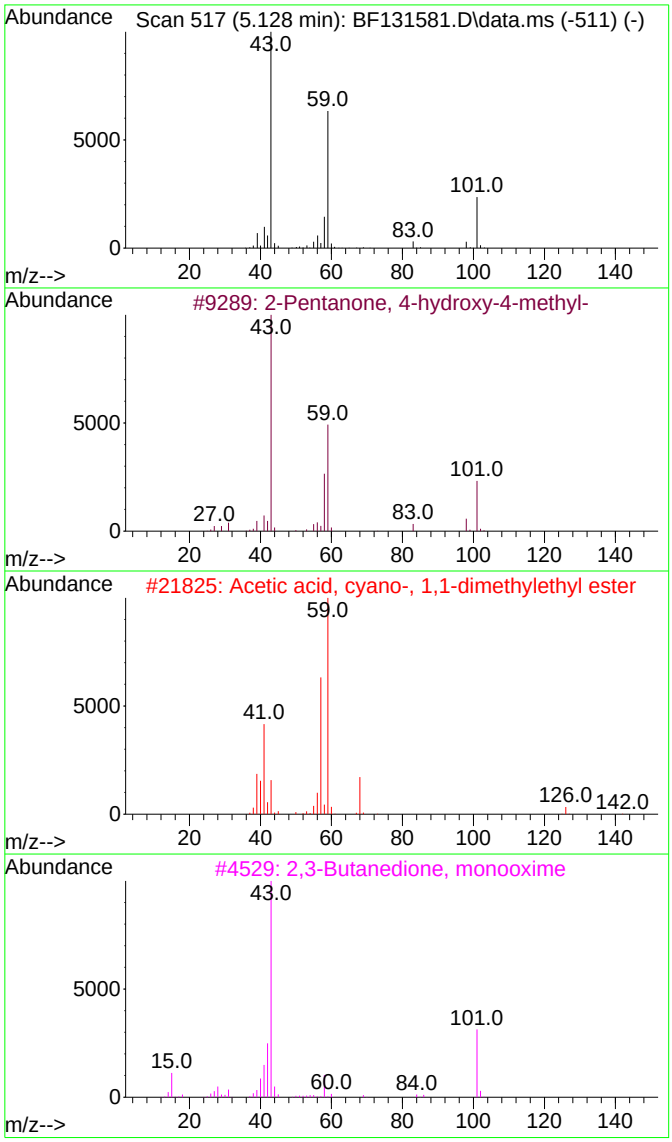
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

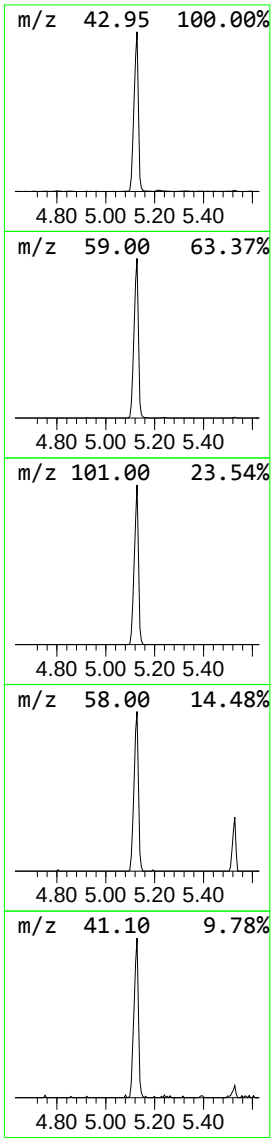
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	33.13 ng	628292	1,4-Dichlorobenzene-d4	6.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131581.D
Acq On : 09 Dec 2022 22:57
Operator : CG\JU
Sample : N5943-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RM-301

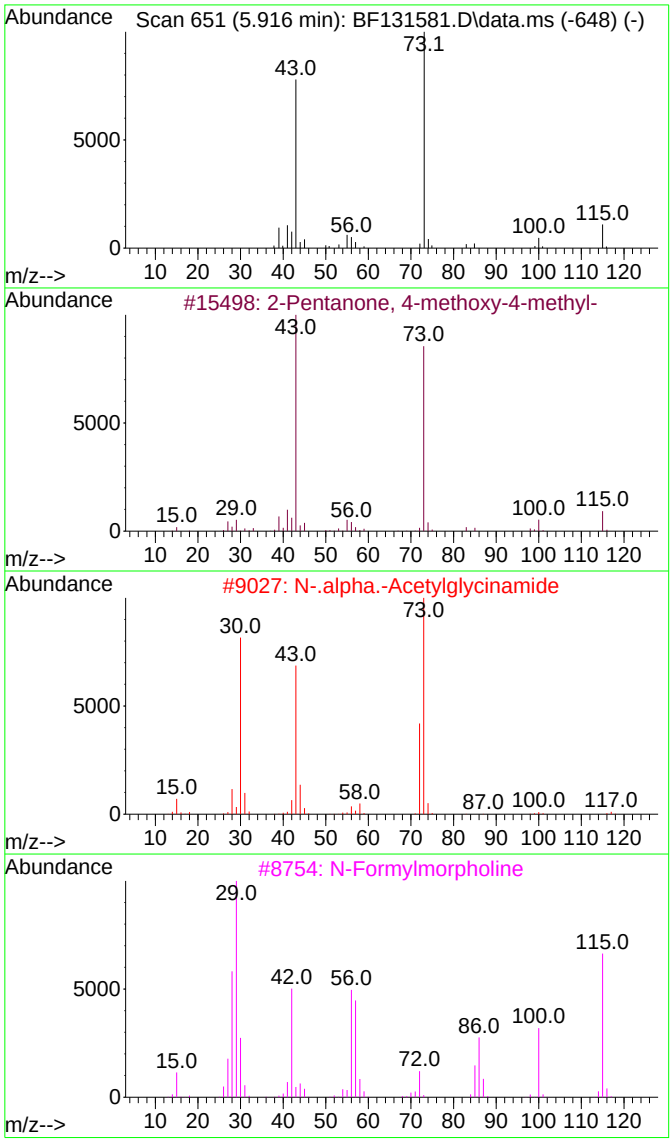
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

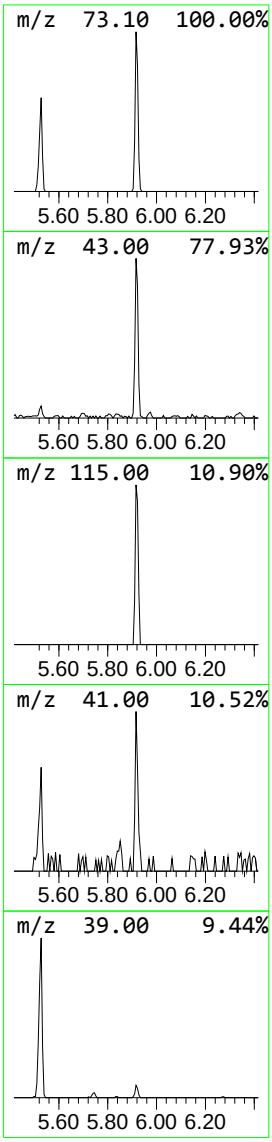
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.916	2.54 ng	48136	1,4-Dichlorobenzene-d4	6.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	47
3	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2-Pentenoic acid, 4-hydroxy-	116	C5H8O3	028525-83-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131581.D
Acq On : 09 Dec 2022 22:57
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Sample : N5943-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

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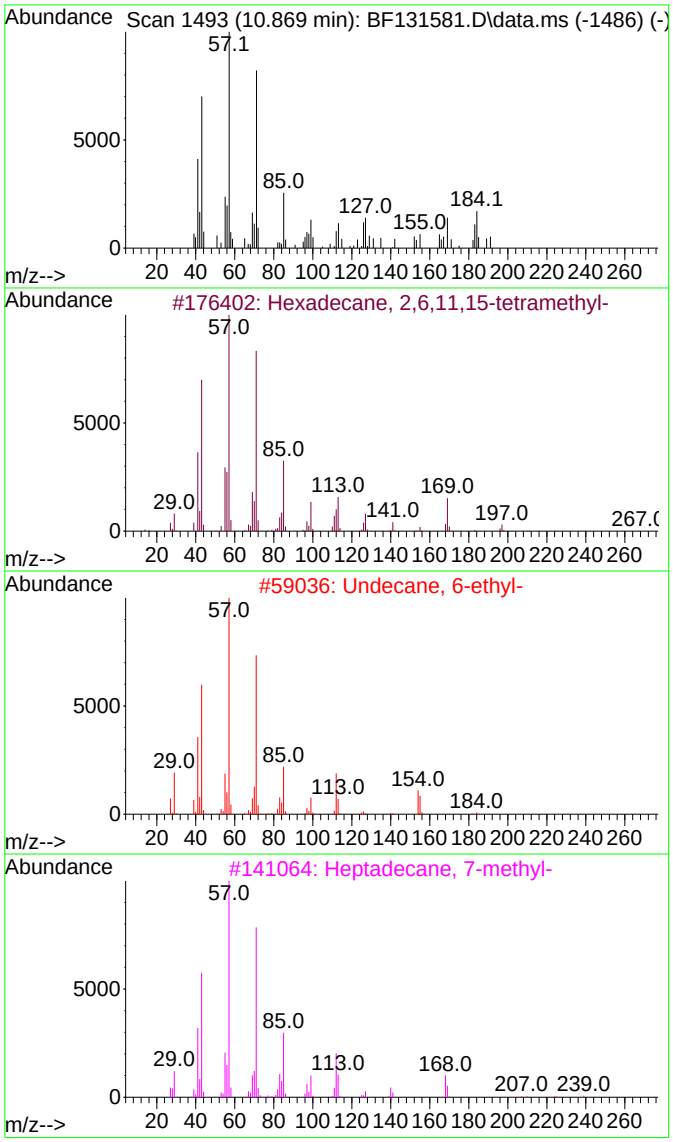
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

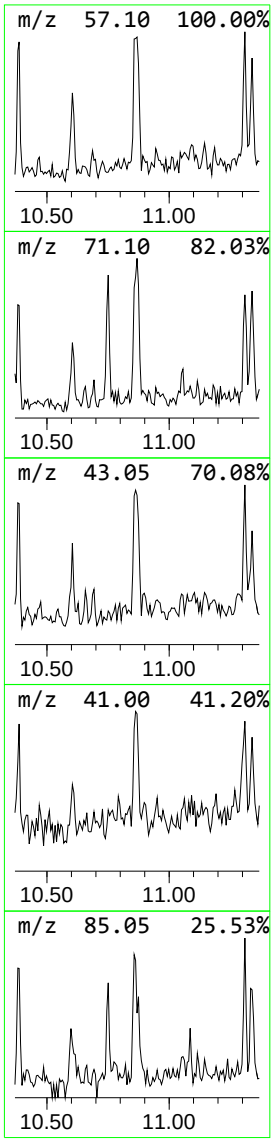
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexadecane, 2,6,11,15-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.869	2.18 ng	42488	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	64
2	Undecane, 6-ethyl-	184	C13H28	017312-60-6	53
3	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	53
4	Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	50
5	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131581.D
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

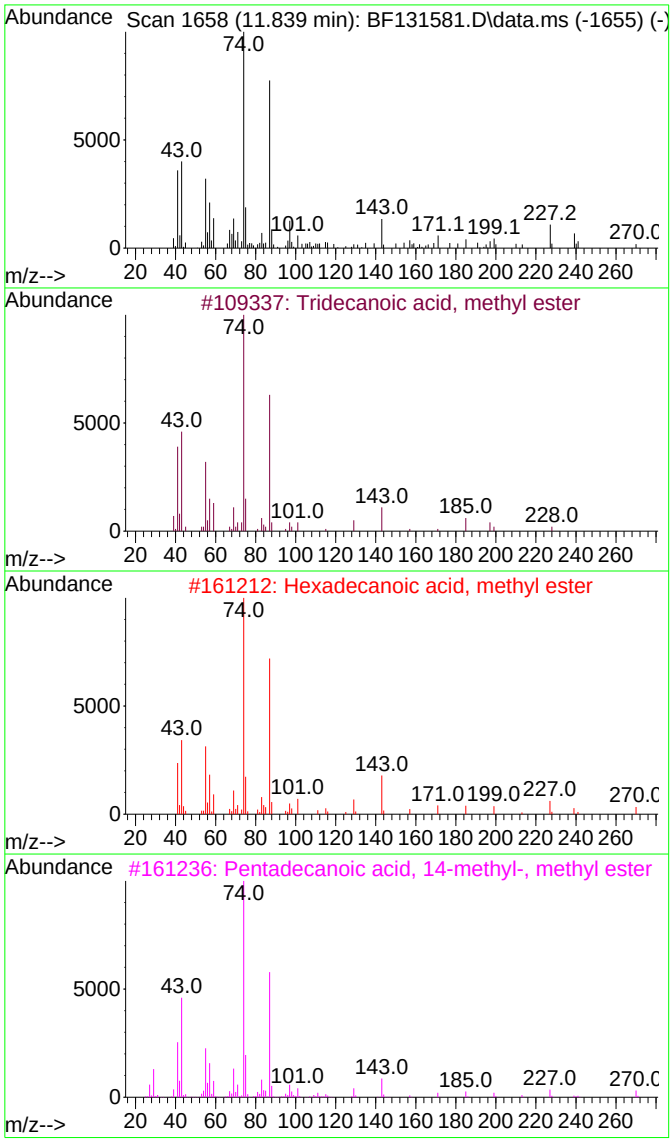
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

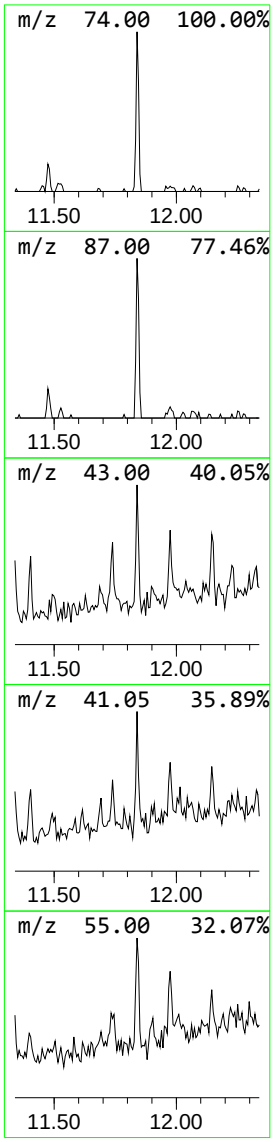
****

Peak Number 6 Tridecanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	2.25 ng	43897	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	80
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	72
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
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ALS Vial : 21 Sample Multiplier: 1

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

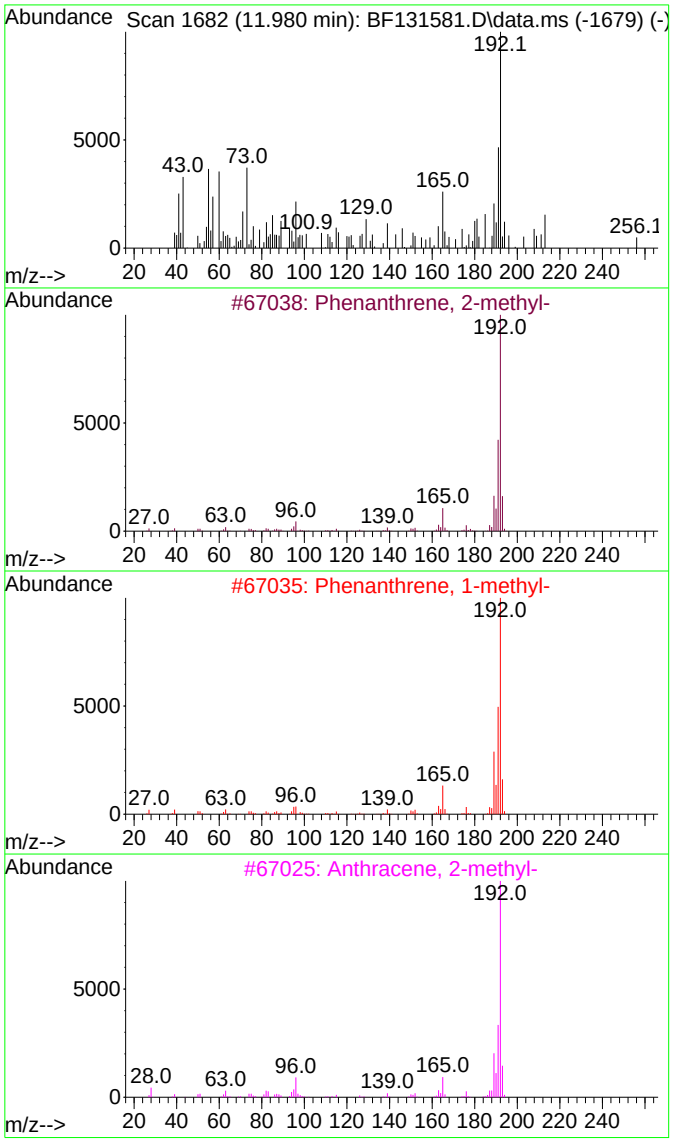
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

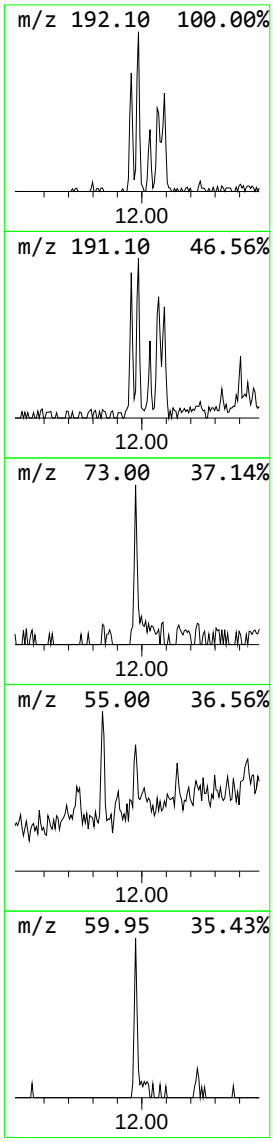
****

Peak Number 7 Phenanthrene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.980	2.59 ng	50559	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	64
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	58
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	58
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	52
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	52





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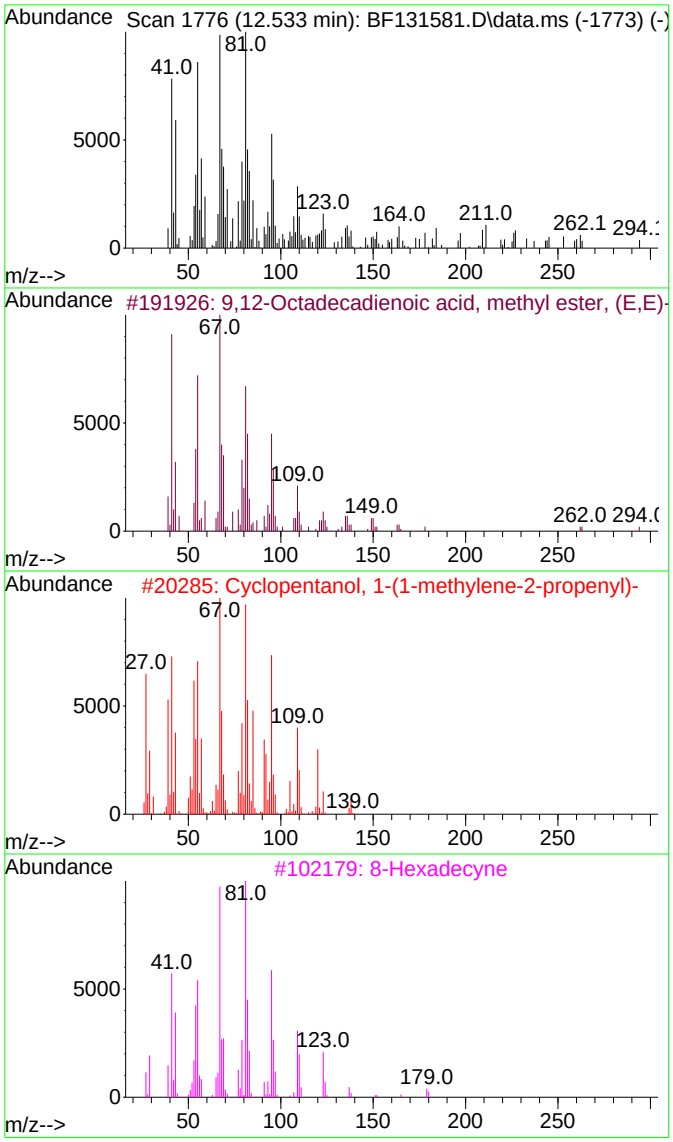
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

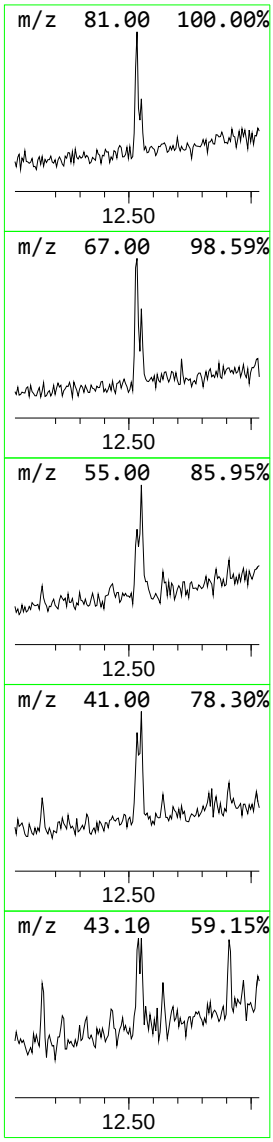
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.533	3.54 ng	69181	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	93
2	Cyclopentanol, 1-(1-methylene-2-...	138	C9H14O	078158-11-9	81
3	8-Hexadecyne	222	C16H30	019781-86-3	74
4	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	70
5	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131581.D
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Operator : CG\JU
Sample : N5943-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

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

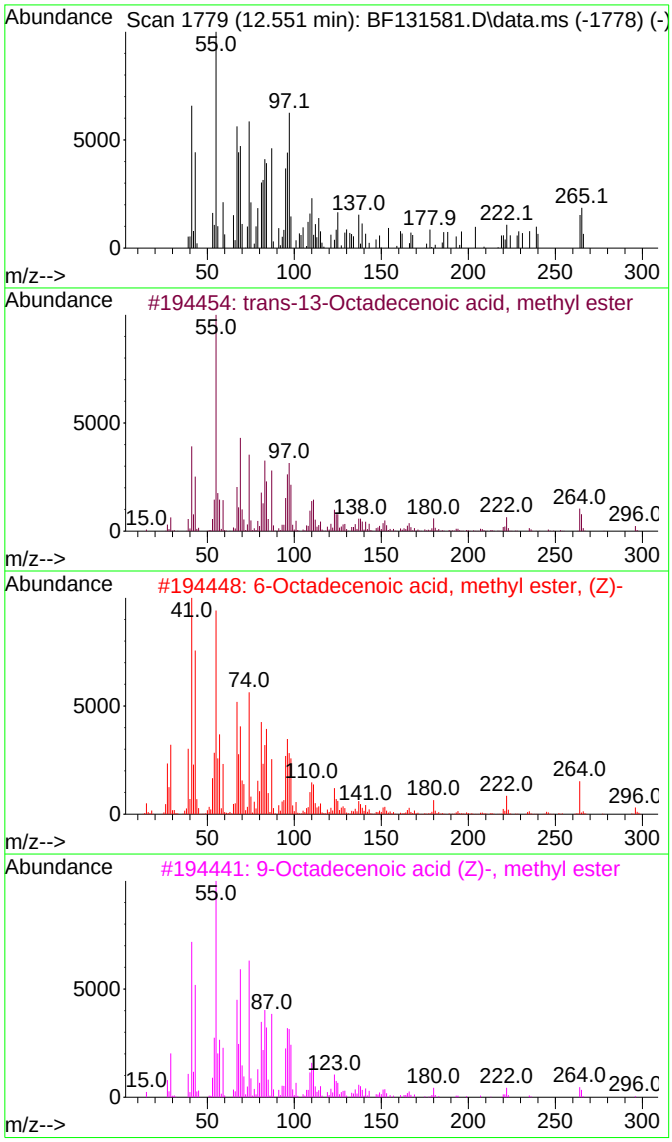
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

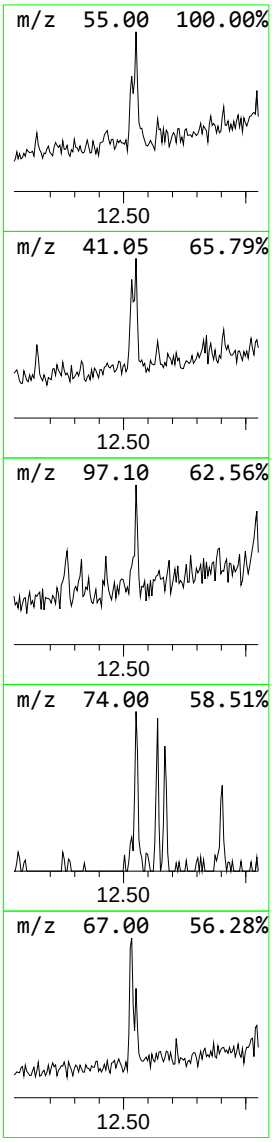
****

Peak Number 9 trans-13-Octadecenoic acid,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	2.55 ng	49766	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	90
2	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	64
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	64
4	Methyl myristoleate	240	C15H28O2	056219-06-8	62
5	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131581.D
Acq On : 09 Dec 2022 22:57
Operator : CG\JU
Sample : N5943-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RM-301

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

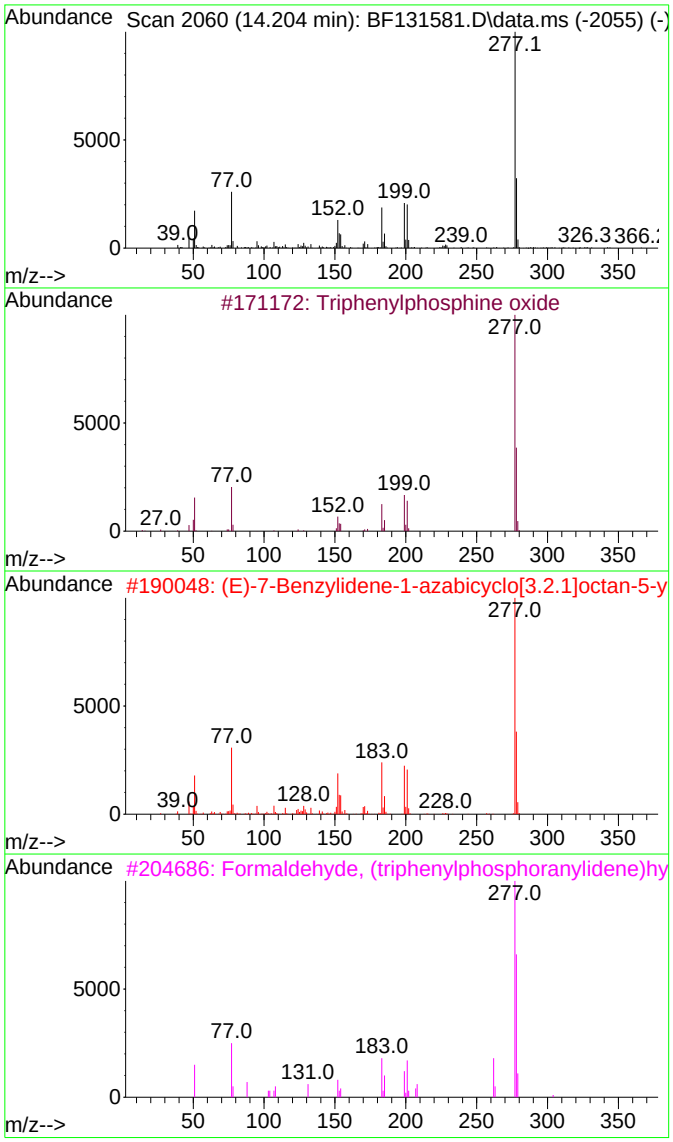
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

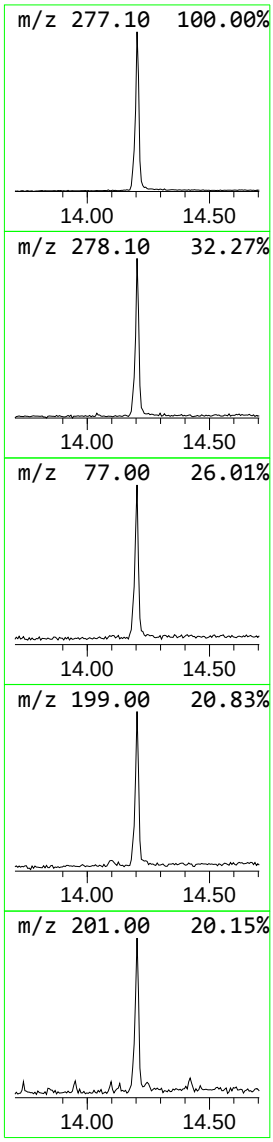
****

Peak Number 10 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.204	15.94 ng	312558	Chrysene-d12	14.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	64
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	46
5	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131581.D
Acq On : 09 Dec 2022 22:57
Operator : CG\JU
Sample : N5943-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RM-301

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...	2.187	28.6	ng	542923	1	6.910	379237	20.0
2-Pentanone, 4-...	5.128	33.1	ng	628292	1	6.910	379237	20.0
2-Pentanone, 4-...	5.916	2.5	ng	48136	1	6.910	379237	20.0
Hexadecane, 2,6...	10.869	2.2	ng	42488	4	11.457	390447	20.0
Tridecanoic aci...	11.839	2.3	ng	43897	4	11.457	390447	20.0
Phenanthrene, 2...	11.980	2.6	ng	50559	4	11.457	390447	20.0
9,12-Octadecadi...	12.533	3.5	ng	69181	4	11.457	390447	20.0
trans-13-Octade...	12.551	2.5	ng	49766	4	11.457	390447	20.0
Triphenylphosph...	14.204	15.9	ng	312558	5	14.110	392215	20.0