LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

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: BF134317.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	499	507	514	rBV2	34623	62476	3.47%	0.398%
2	5.469	571	575	583	rBV	1577242	1520559	84.51%	9.686%
3	5.857	635	641	645	rVB3	15913	25553	1.42%	0.163%
4	5.993	660	664	668	rVB3	16768	22306	1.24%	0.142%
5	6.087	674	680	686	rBV4	25360	45905	2.55%	0.292%
6	6.275	707	712	714	rBV3	17476	23362	1.30%	0.149%
7	6.363	724	727	735	rBV3	33849	44539	2.48%	0.284%
8	6.475	742	746	758	rVB	1642817	1519956	84.48%	9.682%
9	6.669	775	779	790	rBV3	53218	95856	5.33%	0.611%
10	6.834	804	807	813	rVB	512015	450419	25.03%	2.869%
11	7.098	847	852	856	rVB3	19236	24484	1.36%	0.156%
12	7.398	899	903	906	rBV	1195554	971134	53.98%	6.186%
13	7.422	906	907	911	rVB2	29834	22268	1.24%	0.142%
14	8.116	1021	1025	1028	rBV	655017	541091	30.07%	3.447%
15	8.528	1092	1095	1097	rBV2	27408	24441	1.36%	0.156%
16	9.134	1195	1198	1204	rBV3	33659	39588	2.20%	0.252%
17	9.192	1204	1208	1211	rBV	2280744	1799208	100.00%	11.461%
18	9.263	1218	1220	1223	rBV3	22713	22321	1.24%	0.142%
19	9.304	1224	1227	1231	rBV3	34398	35606	1.98%	0.227%
20	9.528	1262	1265	1267	rBV2	22810	22529	1.25%	0.144%
21	9.587	1271	1275	1278	rVB2	35236	43931	2.44%	0.280%
22	9.734	1294	1300	1304	rBV6	28348	46196	2.57%	0.294%
23	9.869	1320	1323	1327	rVB	632467	546356	30.37%	3.480%
24	10.075	1353	1358	1362	rBV3	54155	70588	3.92%	0.450%
25	10.275	1389	1392	1394	rBV4	22131	24348	1.35%	0.155%
26	10.422	1413	1417	1423	rBV2	28300	38915	2.16%	0.248%
27	10.522	1431	1434	1439	rVB3	23962	34275	1.91%	0.218%
28	10.575	1441	1443	1447	rVB5	19912	22679	1.26%	0.144%
29	10.663	1455	1458	1468	rBV	1147494	1012489	56.27%	6.450%
30	10.786	1474	1479	1482	rBV2	54945	72467	4.03%	0.462%
31	11.028	1517	1520	1523	rVB5	21379	25726	1.43%	0.164%
32	11.257	1556	1559	1565	rVB2	42521	50827	2.82%	0.324%
33	11.369	1574	1578	1580	rBV	566093	537088	29.85%	3.421%
34	11.386	1580	1581	1585	rVV	175811	152829	8.49%	0.974%
35	11.445	1588	1591	1593	rVB	33228	33029	1.84%	0.210%
36	11.898	1661	1668	1679	rBV	803210	1115334	61.99%	7.105%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

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	11.980	1680	1682	1685	rVV	44990	39796	2.21%	0.254%
38	12.422	1755	1757	1760	rBV	32540	33859	1.88%	0.216%
39	12.469	1760	1765	1770	rVB6	38596	73278	4.07%	0.467%
40	12.586	1782	1785	1788	rBV	331218	316351	17.58%	2.015%
41	12.686	1798	1802	1808	rBV	446340	518873	28.84%	3.305%
42	12.822	1819	1825	1830	rBV	242252	294630	16.38%	1.877%
43	12.963	1845	1849	1856	rVB	1795655	1548890	86.09%	9.867%
44	13.851	1997	2000	2003	rBV	122099	185473	10.31%	1.181%
45	13.886	2003	2006	2013	rVB	651802	703459	39.10%	4.481%
46	14.027	2026	2030	2033	rBV2	445077	495448	27.54%	3.156%
47	15.539	2283	2287	2294	rVB	234612	347607	19.32%	2.214%

Sum of corrected areas: 15698342

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
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Acq On : 17 Jul 2023 15:50
Operator : CG\JU
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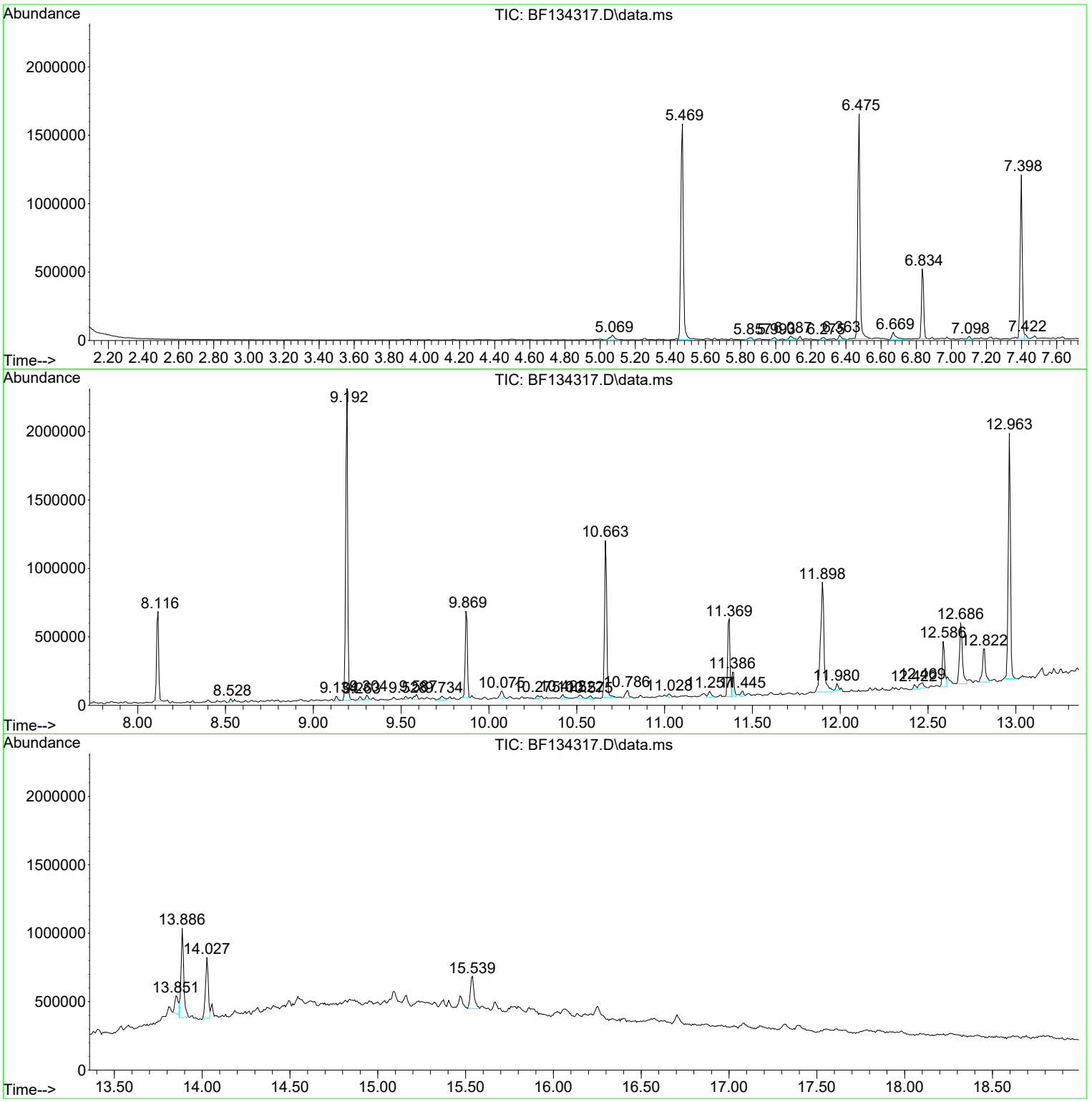
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

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\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

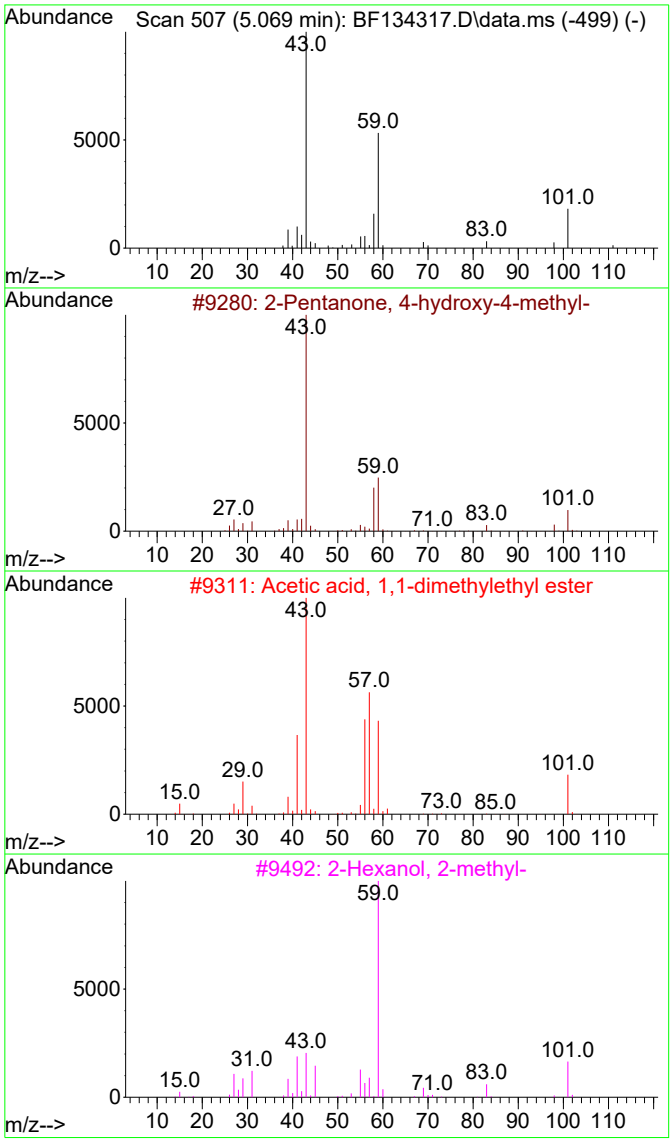
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

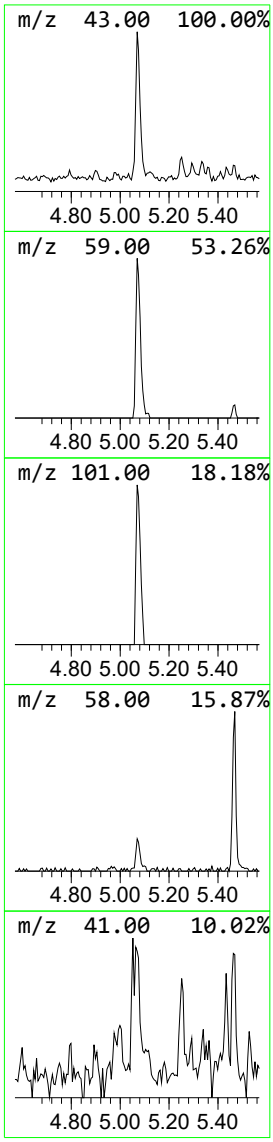
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	2.77 ng	62476	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

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

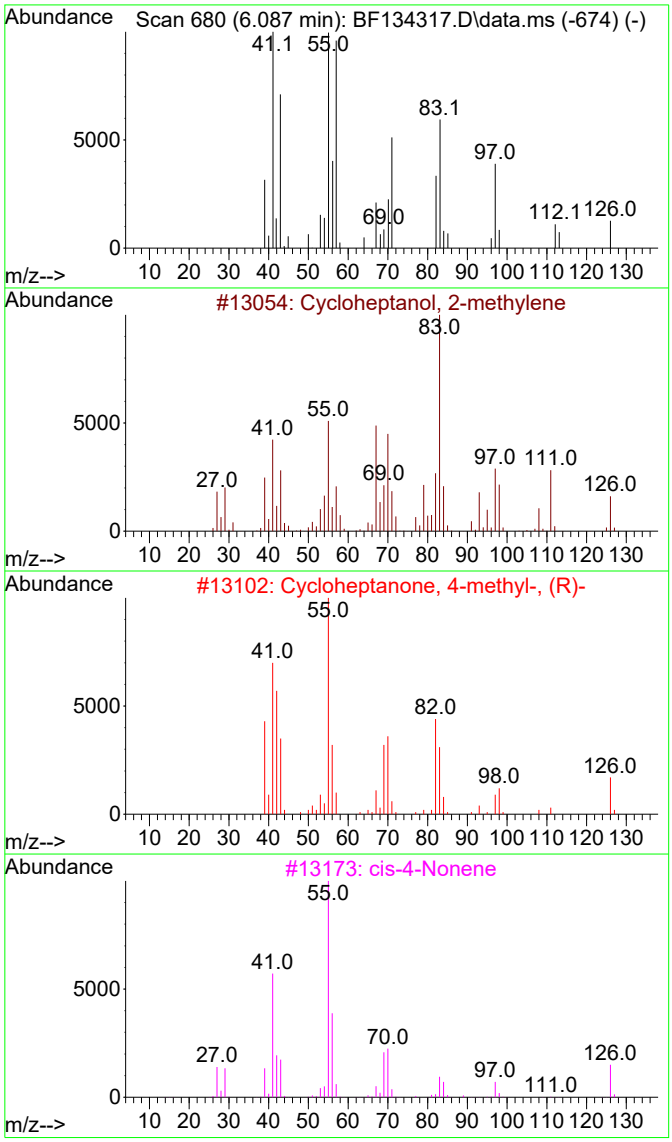
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

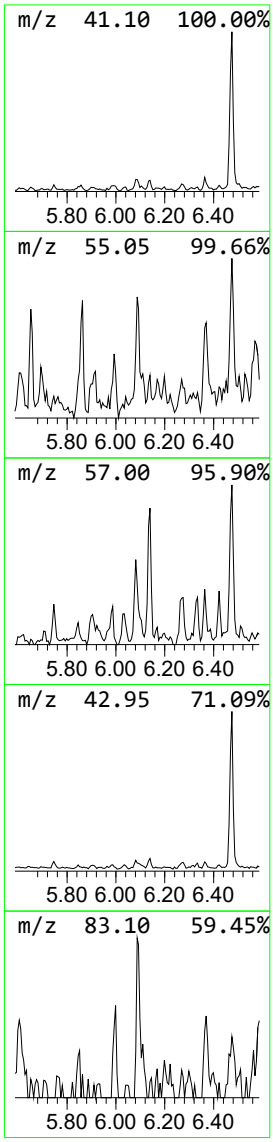
****

Peak Number 2 unknown6.087 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.087	2.04 ng	45905	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptanol, 2-methylene	126	C8H14O	016240-38-3	27
2	Cycloheptanone, 4-methyl-, (R)-	126	C8H14O	013609-59-1	27
3	cis-4-Nonene	126	C9H18	010405-84-2	25
4	2-Nonene	126	C9H18	002216-38-8	25
5	Cyclohexane, propyl-	126	C9H18	001678-92-8	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

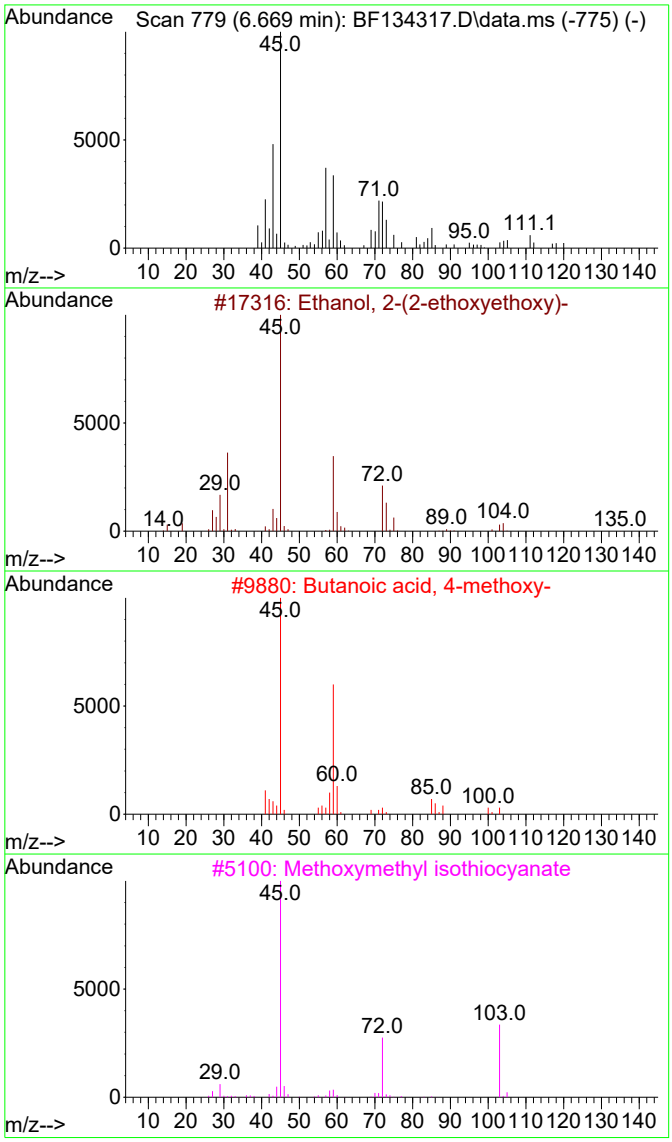
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

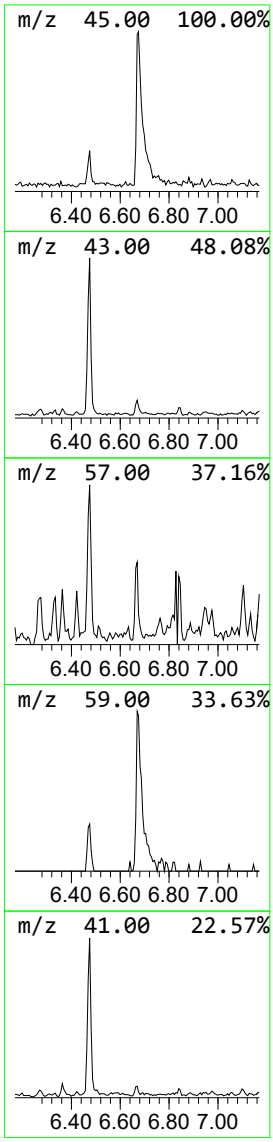
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.669	4.26 ng	95856	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	59
2	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	47
3	Methoxymethyl isothiocyanate	103	C3H5NOS	019900-84-6	47
4	Methane, tert-butoxymethoxy-	118	C6H14O2	024209-75-4	38
5	2-Nonanol	144	C9H20O	000628-99-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

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

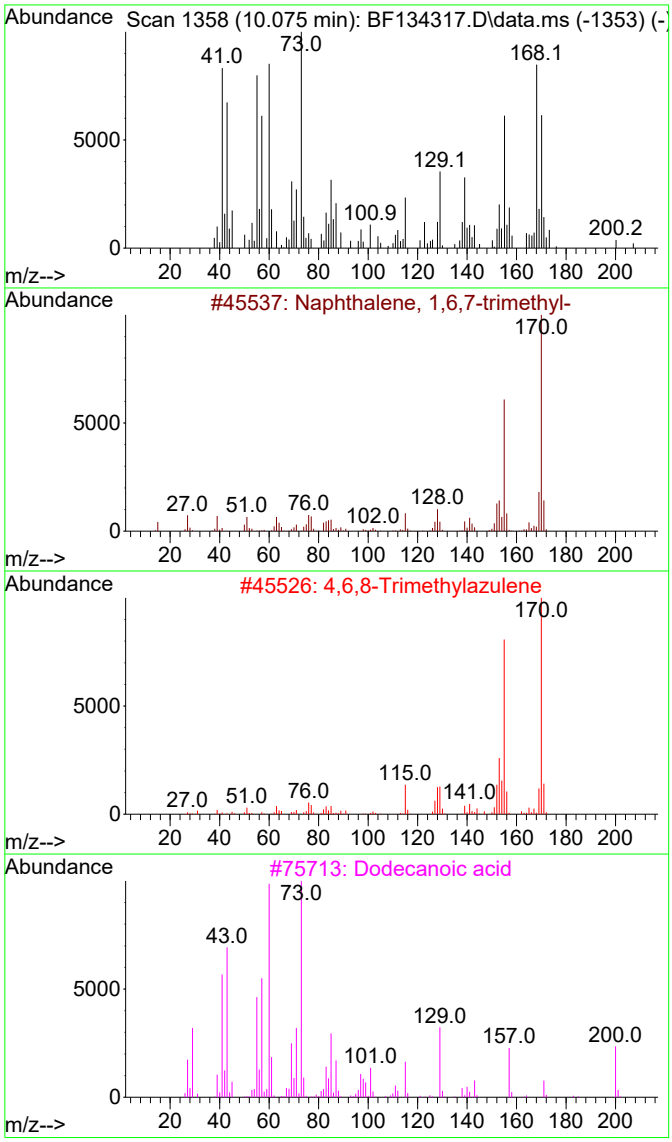
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

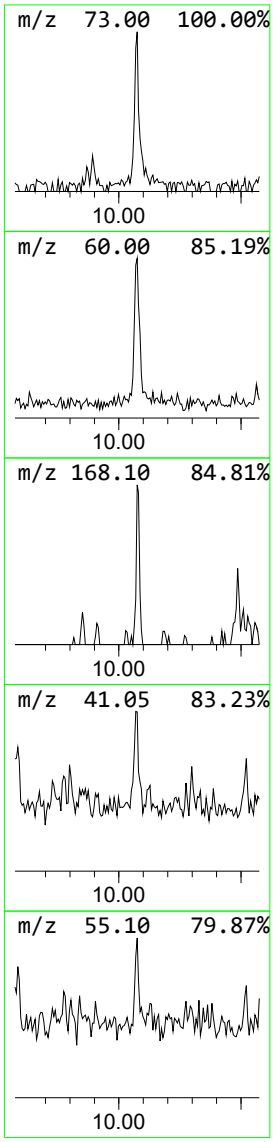
****

Peak Number 4 unknown10.075 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.075	2.58 ng	70588	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	38
2	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	38
3	Dodecanoic acid	200	C12H24O2	000143-07-7	38
4	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	35
5	3-(2-Methyl-propenyl)-1H-indene	170	C13H14	1000187-78-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

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

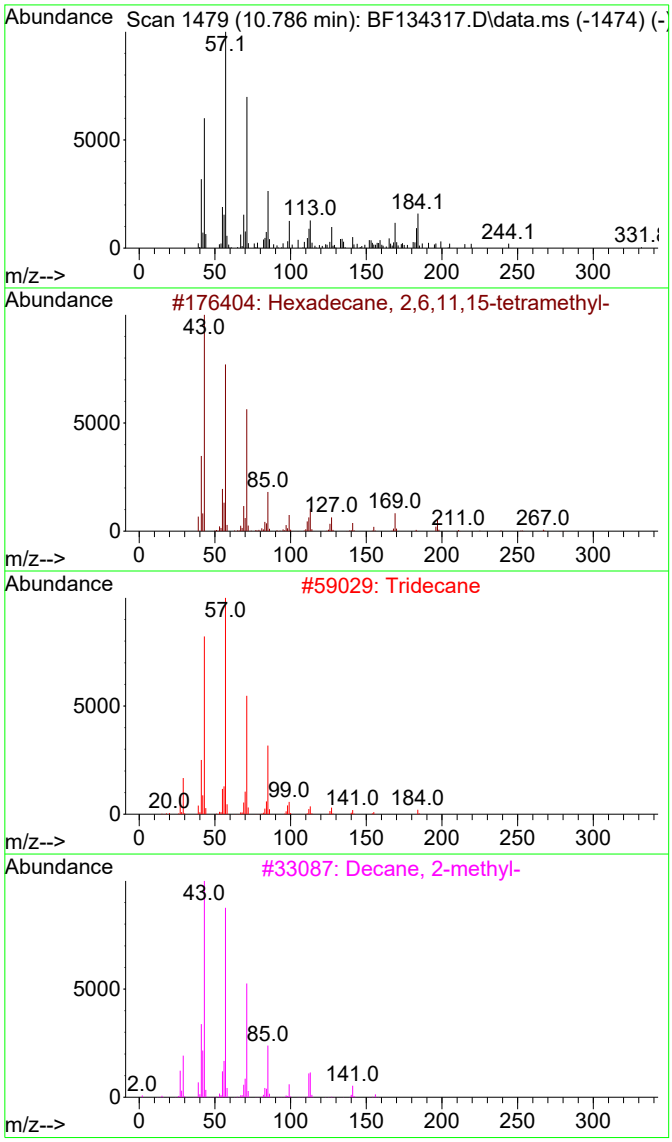
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

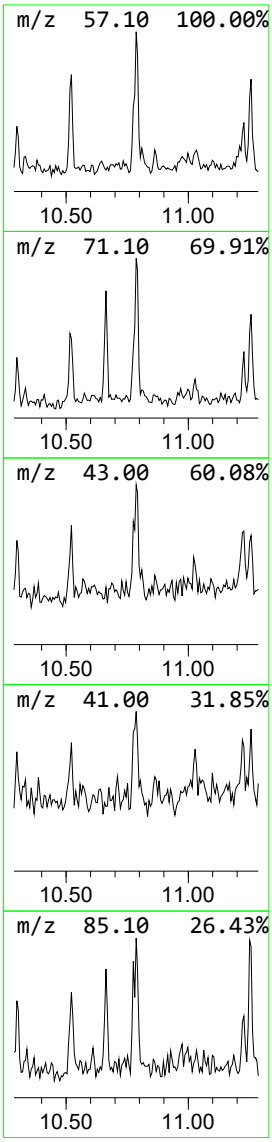
****

Peak Number 5 Hexadecane, 2,6,11,15-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.786	2.70 ng	72467	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	83
2	Tridecane	184	C13H28	000629-50-5	58
3	Decane, 2-methyl-	156	C11H24	006975-98-0	52
4	Heneicosane	296	C21H44	000629-94-7	50
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

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

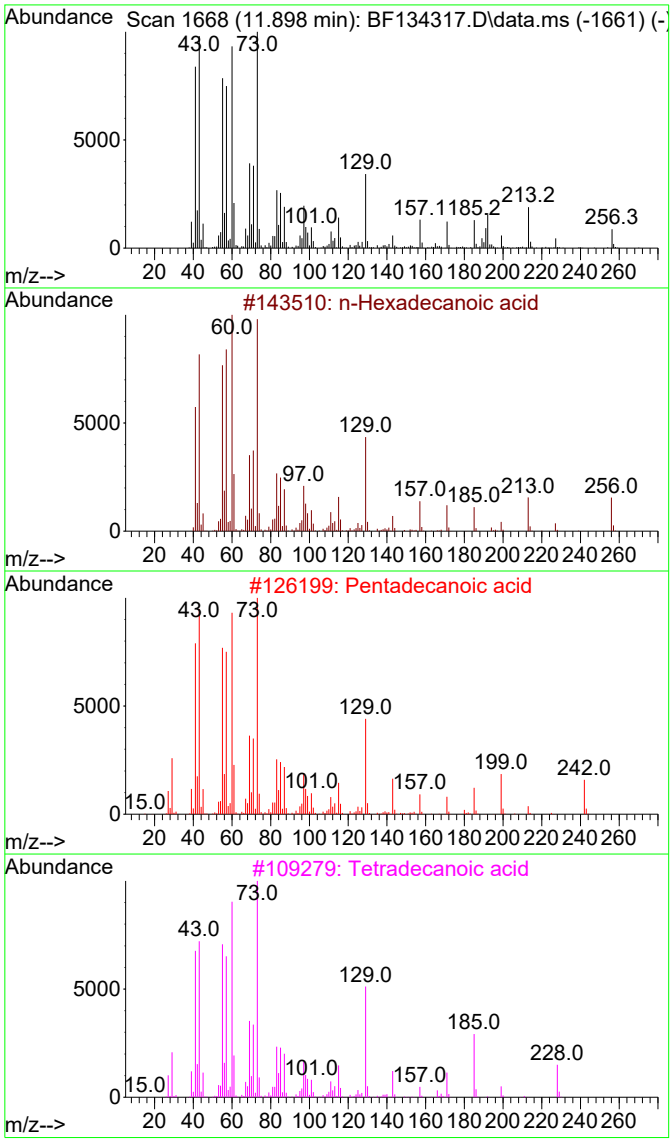
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

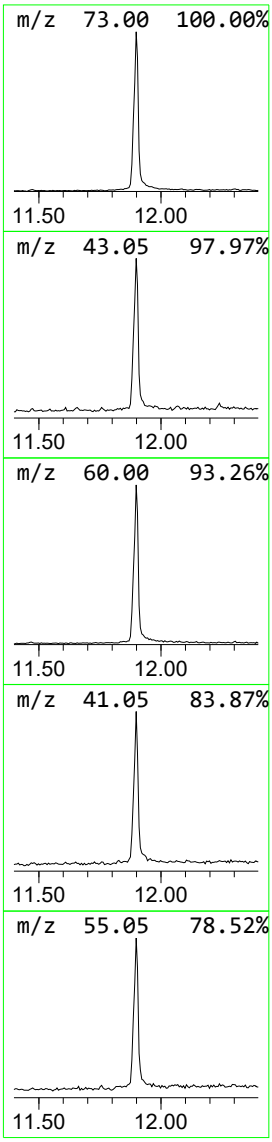
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	41.53 ng	1115330	Phenanthrene-d10	11.369

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

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

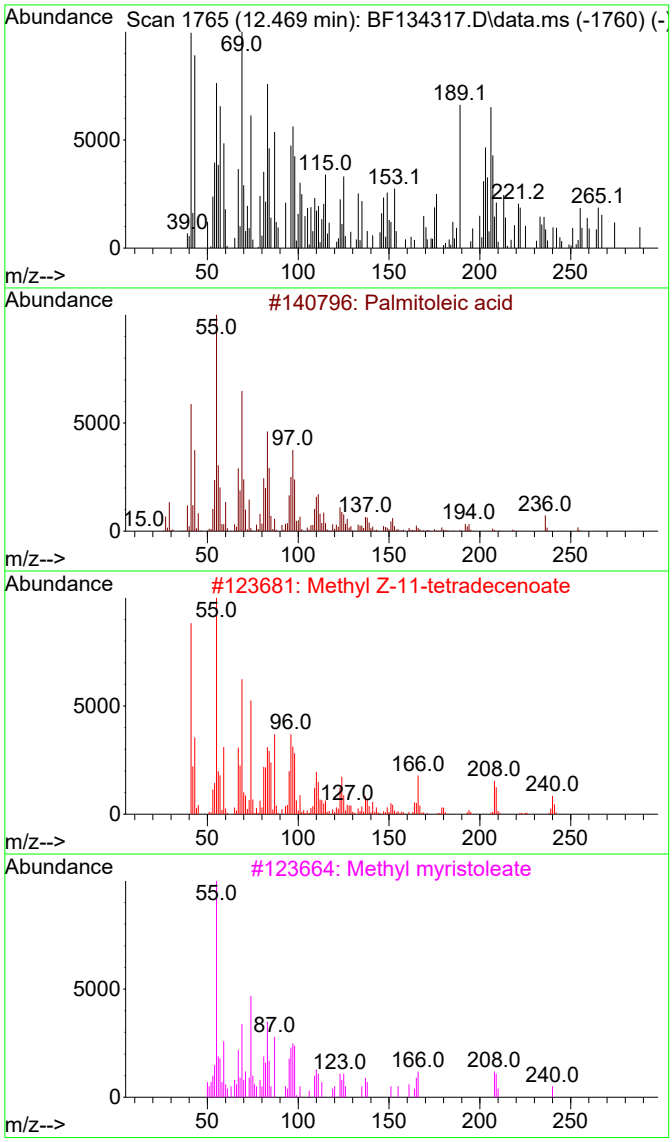
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

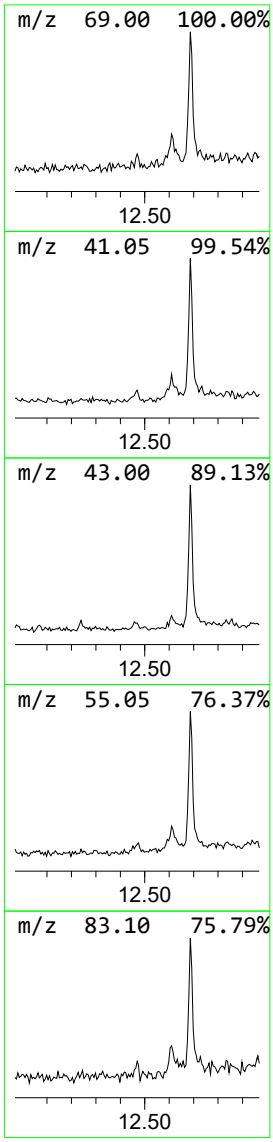
****

Peak Number 7 Palmitoleic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	2.73 ng	73278	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	52
2	Methyl Z-11-tetradecenoate	240	C15H28O2	1000130-82-8	46
3	Methyl myristoleate	240	C15H28O2	056219-06-8	46
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	43
5	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

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

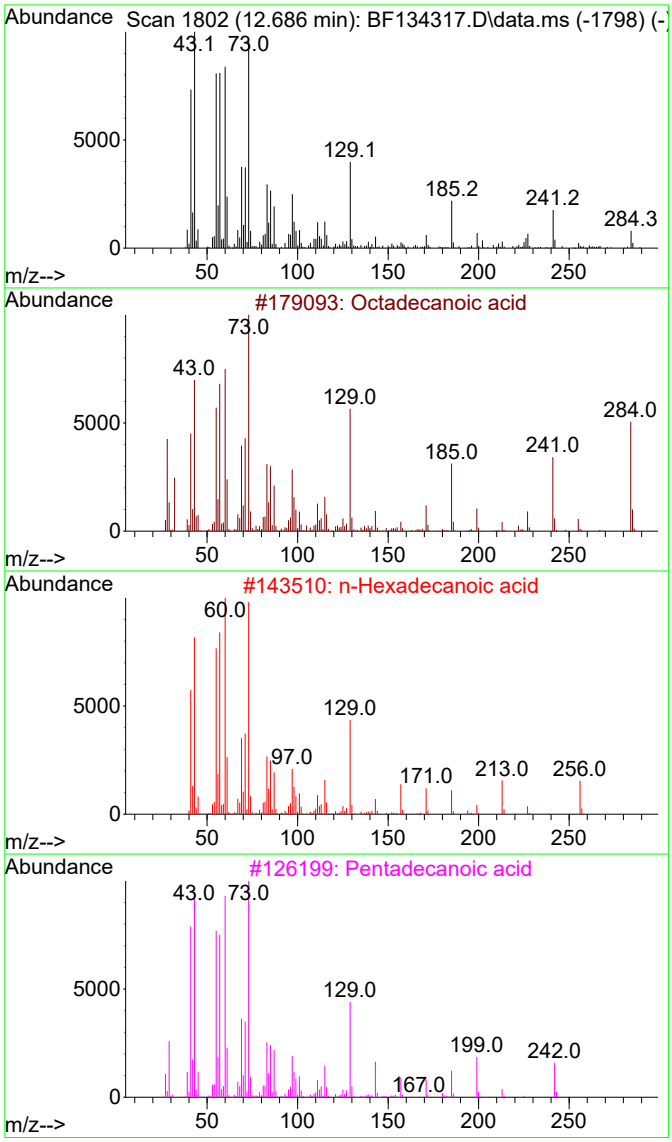
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

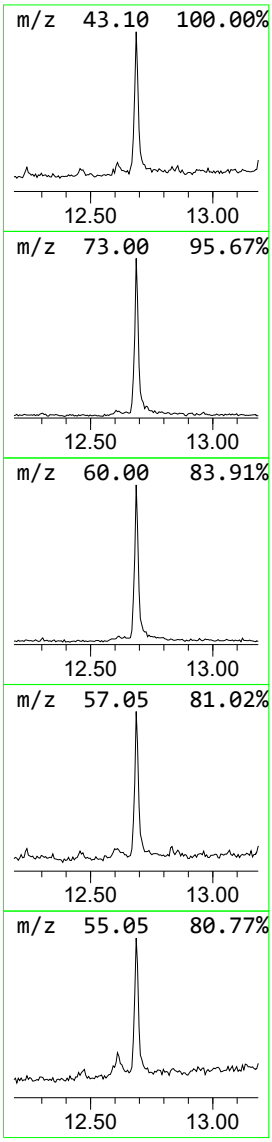
****

Peak Number 8 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	19.32 ng	518873	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





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Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

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

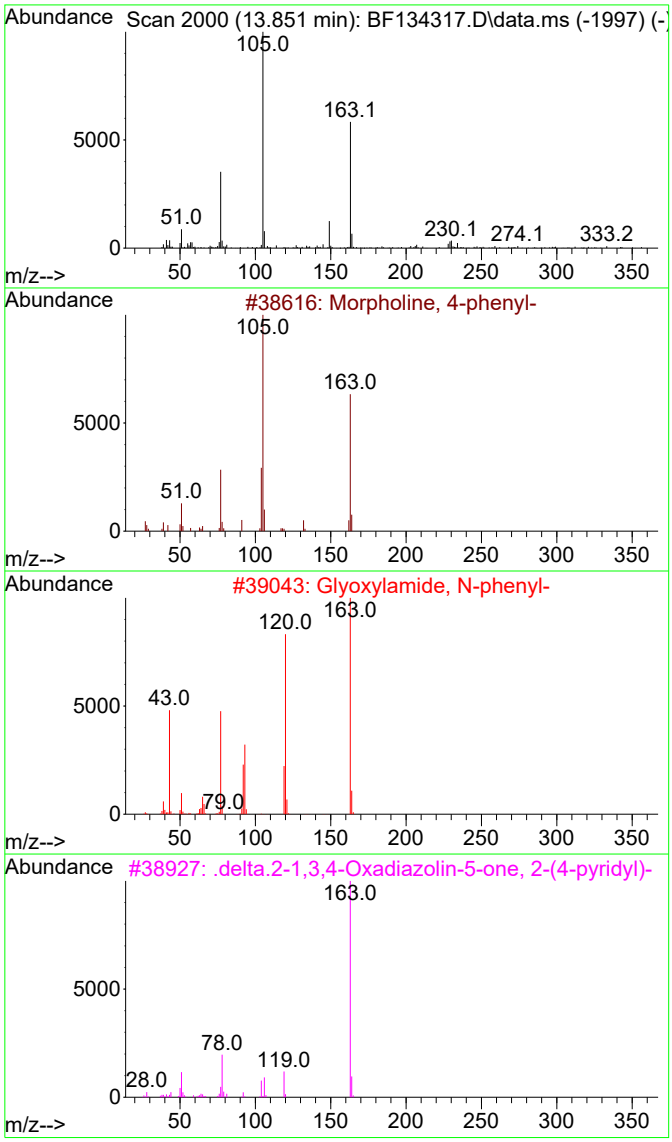
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

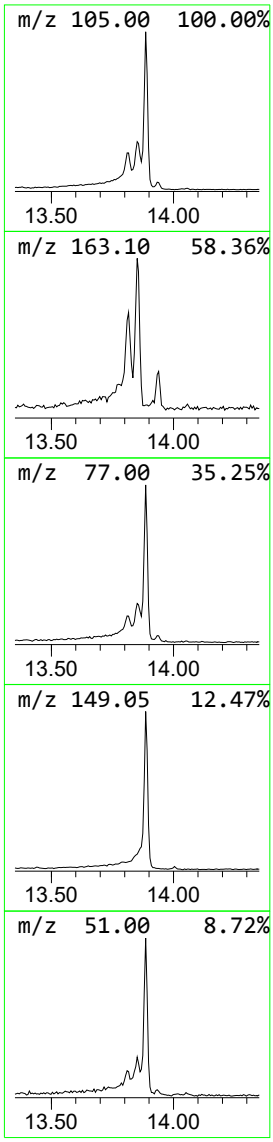
****

Peak Number 9 Morpholine, 4-phenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	7.49 ng	185473	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	43
3	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	35
4	p-(N-benzoylamino-N'-methyl)benz...	290	C14H14N2O3S	1000395-68-9	30
5	1,2-Ethanediol, dibenzoate	270	C16H14O4	000094-49-5	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

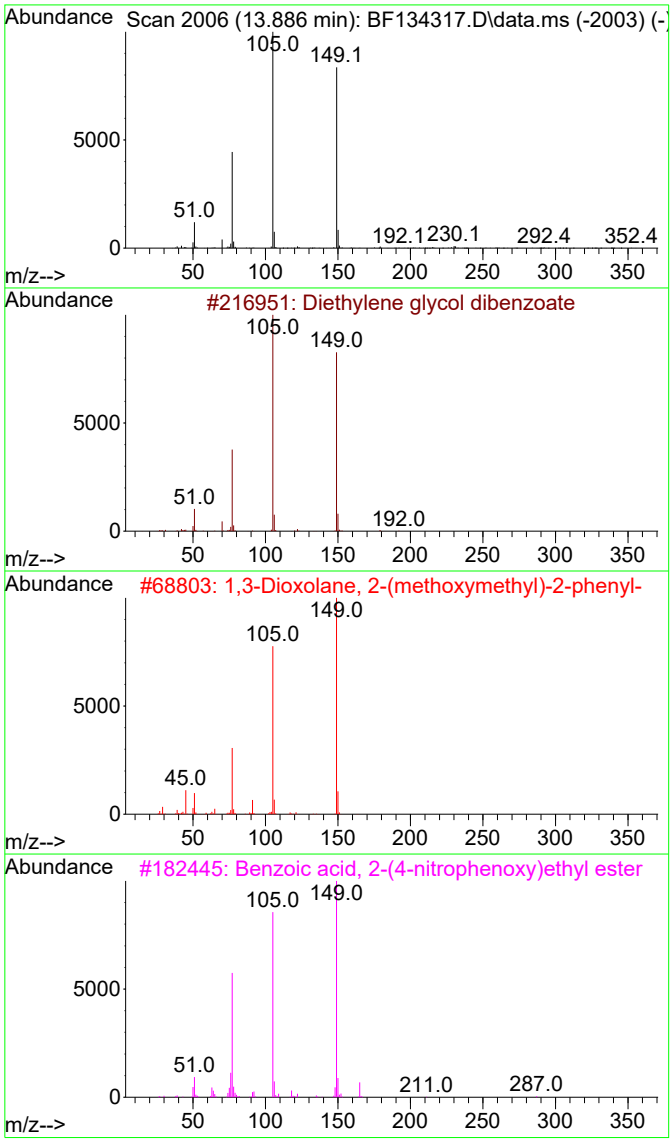
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

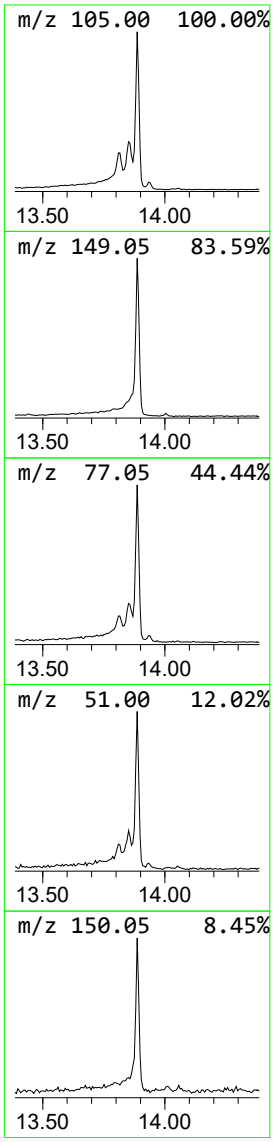
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	28.40 ng	703459	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
3	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
4	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52
5	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134317.D
Acq On : 17 Jul 2023 15:50
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

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
2-Pentanone, 4-...	5.069	2.8	ng	62476	1	6.834	450419	20.0
unknown6.087	6.087	2.0	ng	45905	1	6.834	450419	20.0
Ethanol, 2-(2-e...	6.669	4.3	ng	95856	1	6.834	450419	20.0
unknown10.075	10.075	2.6	ng	70588	3	9.869	546356	20.0
Hexadecane, 2,6...	10.786	2.7	ng	72467	4	11.369	537088	20.0
n-Hexadecanoic ...	11.898	41.5	ng	1115330	4	11.369	537088	20.0
Palmitoleic acid	12.469	2.7	ng	73278	4	11.369	537088	20.0
Octadecanoic acid	12.686	19.3	ng	518873	4	11.369	537088	20.0
Morpholine, 4-p...	13.851	7.5	ng	185473	5	14.027	495448	20.0
Diethylene glyc...	13.886	28.4	ng	703459	5	14.027	495448	20.0