LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136799.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	7	12	16	rVB2	14194	18197	1.34%	0.179%
2	4.387	387	391	399	rBV	75721	87776	6.47%	0.865%
3	5.022	492	499	502	rBV	951034	1201989	88.59%	11.852%
4	5.422	563	567	582	rBV	611599	596667	43.98%	5.883%
5	6.422	733	737	753	rBV	1038242	883999	65.16%	8.716%
6	6.781	794	798	801	rBV	481798	384549	28.34%	3.792%
7	7.339	888	893	896	rBV	831505	707532	52.15%	6.976%
8	8.057	1010	1015	1018	rBV	610789	491462	36.22%	4.846%
9	9.133	1193	1198	1201	rBV	1666874	1356733	100.00%	13.378%
10	9.816	1310	1314	1323	rBV	576210	524053	38.63%	5.167%
11	9.916	1326	1331	1338	rVB4	11587	16331	1.20%	0.161%
12	10.604	1445	1448	1460	rBV	264901	240421	17.72%	2.371%
13	11.304	1563	1567	1573	rBV	627701	521027	38.40%	5.137%
14	11.839	1654	1658	1662	rBV	48012	59657	4.40%	0.588%
15	12.292	1732	1735	1738	rBV3	16351	16862	1.24%	0.166%
16	12.404	1751	1754	1756	rBV	28644	27370	2.02%	0.270%
17	12.504	1768	1771	1775	rBV5	18526	28776	2.12%	0.284%
18	12.539	1775	1777	1783	rVV6	14869	26728	1.97%	0.264%
19	12.621	1788	1791	1792	rBV3	19600	21475	1.58%	0.212%
20	12.751	1811	1813	1815	rBV3	24150	20003	1.47%	0.197%
21	12.774	1815	1817	1819	rBV2	29855	25978	1.91%	0.256%
22	12.904	1834	1839	1842	rBV	1439449	1305799	96.25%	12.875%
23	12.986	1850	1853	1855	rBV3	29106	33247	2.45%	0.328%
24	13.127	1875	1877	1881	rVB2	38999	46082	3.40%	0.454%
25	13.174	1882	1885	1889	rBV4	51349	77608	5.72%	0.765%
26	13.263	1897	1900	1903	rVB2	65084	63601	4.69%	0.627%
27	13.345	1910	1914	1919	rBV5	48552	109058	8.04%	1.075%
28	13.598	1954	1957	1963	rVB4	68084	107601	7.93%	1.061%
29	13.786	1986	1989	1991	rBV2	93913	114893	8.47%	1.133%
30	13.963	2015	2019	2023	rVB	452358	397309	29.28%	3.918%
31	14.227	2062	2064	2071	rVB2	58741	81297	5.99%	0.802%
32	14.533	2113	2116	2121	rVB4	38037	53641	3.95%	0.529%
33	14.745	2150	2152	2155	rVB2	30947	25232	1.86%	0.249%
34	14.815	2162	2164	2170	rVB4	27023	28742	2.12%	0.283%
35	15.086	2207	2210	2214	rVB	24750	25843	1.90%	0.255%
36	15.439	2265	2270	2284	rVB	292719	414234	30.53%	4.084%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

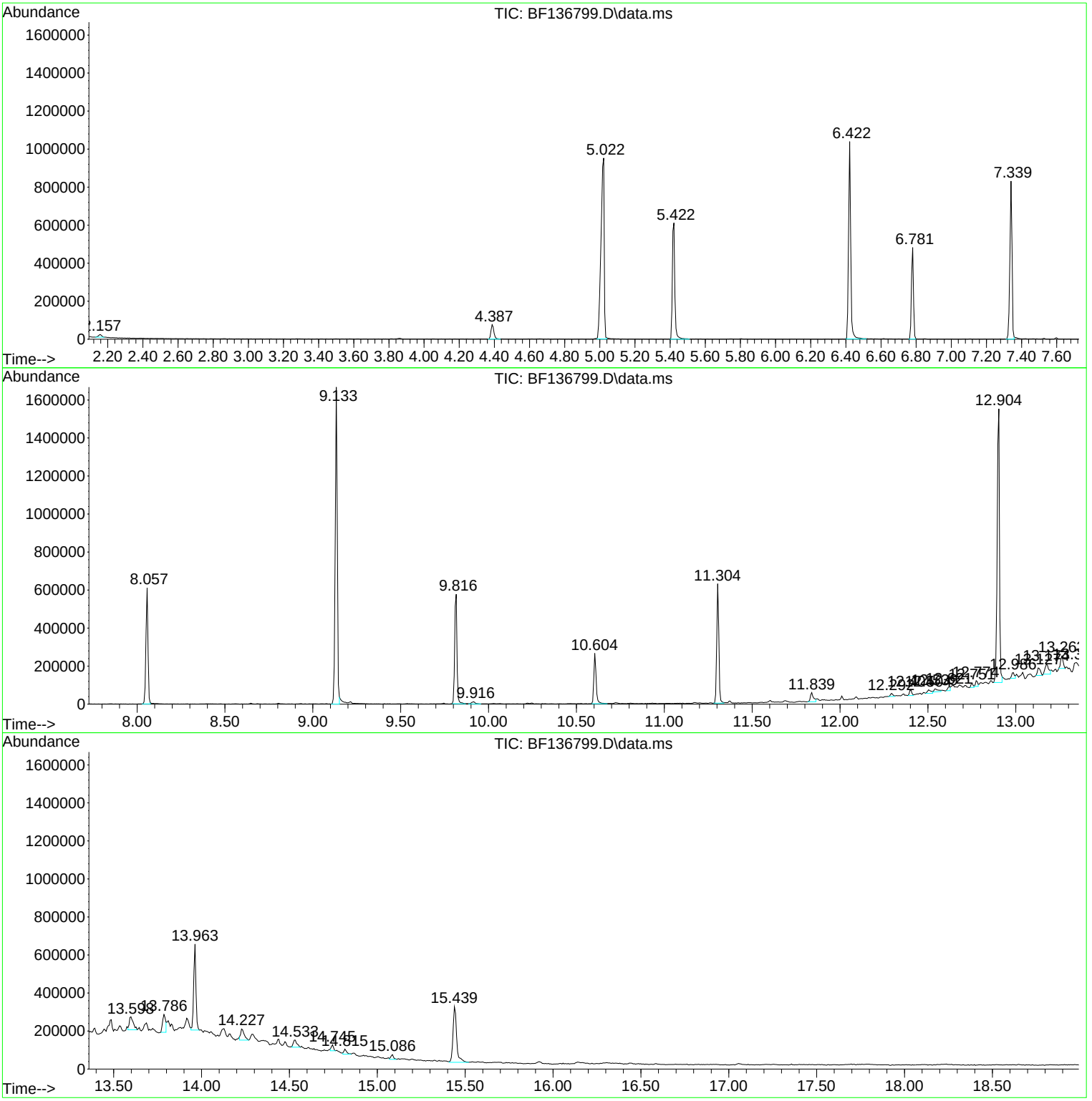
Sum of corrected areas: 10141772

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

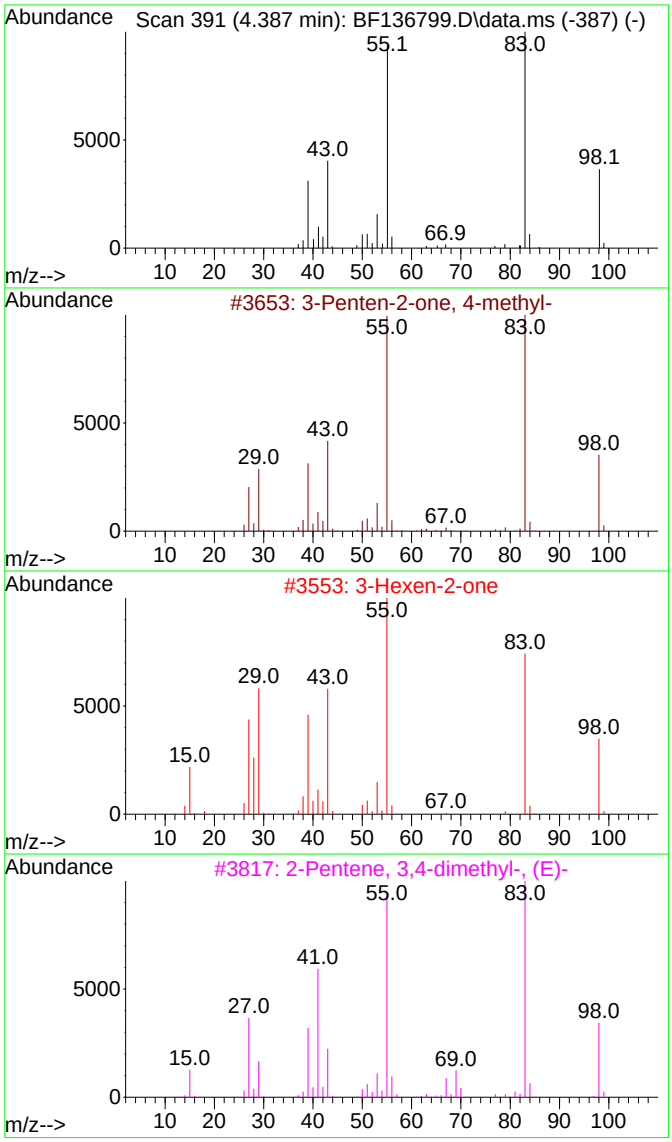
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

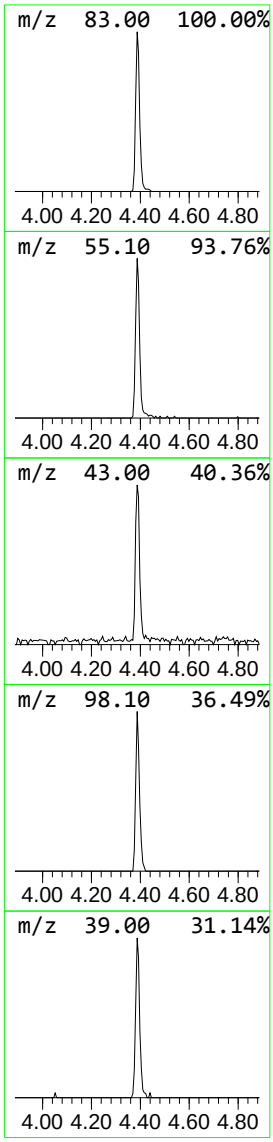
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.387	4.57 ng	87776	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86





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Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

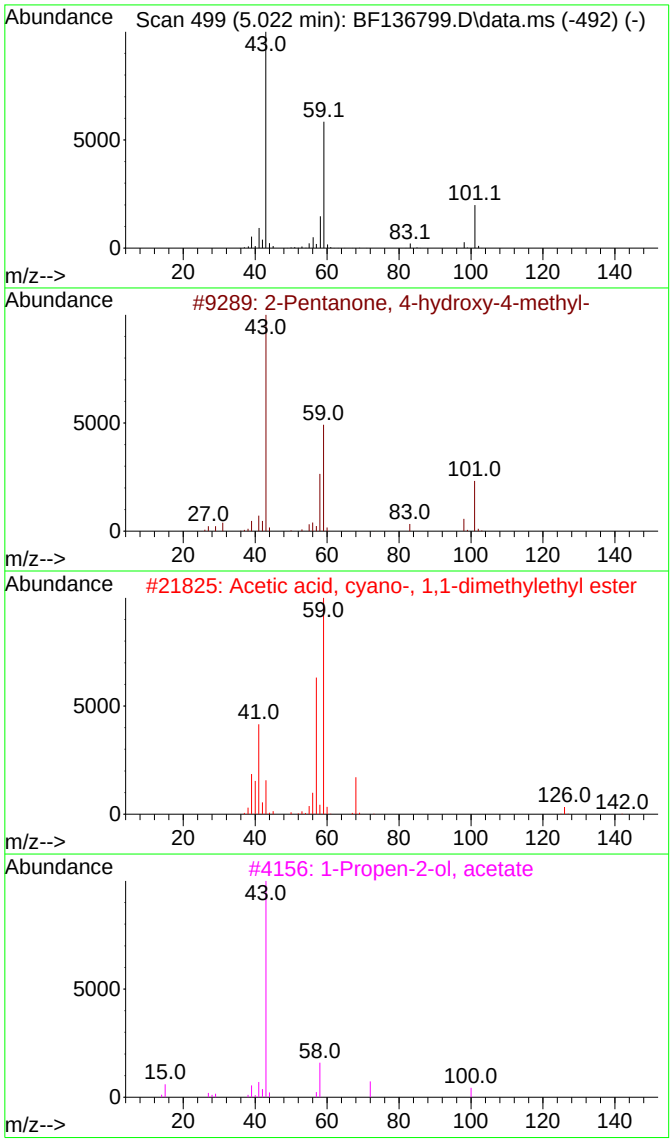
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

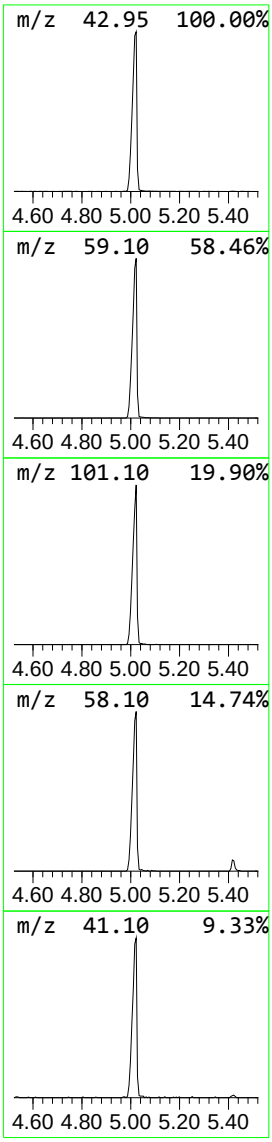
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	62.51 ng	1201990	1,4-Dichlorobenzene-d4	6.781

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	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

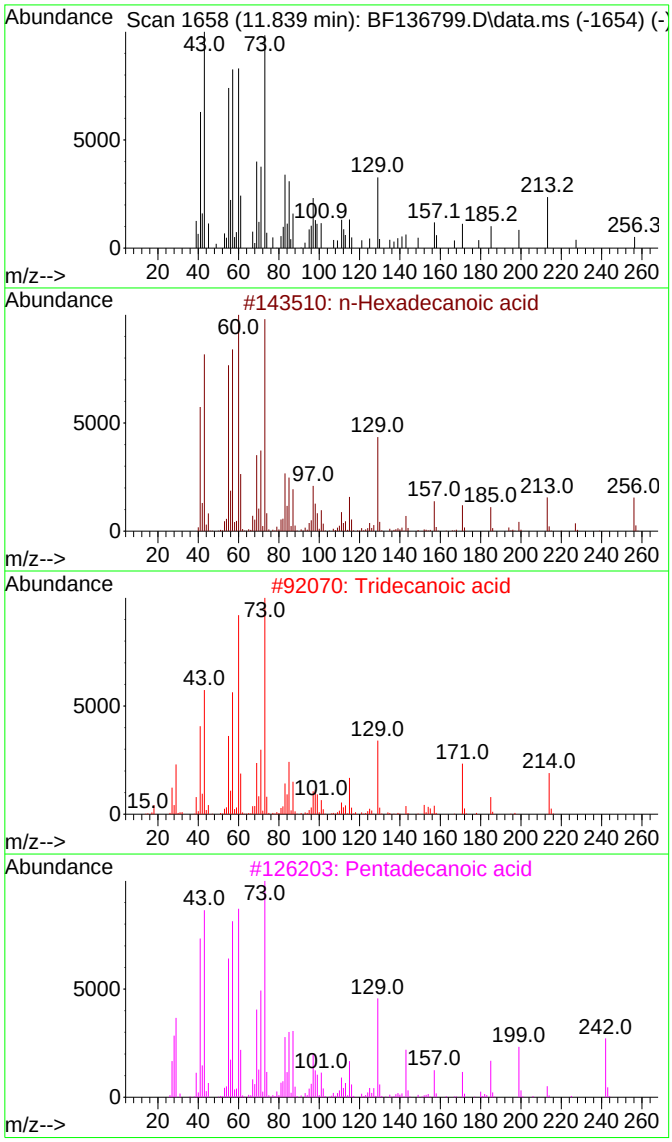
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

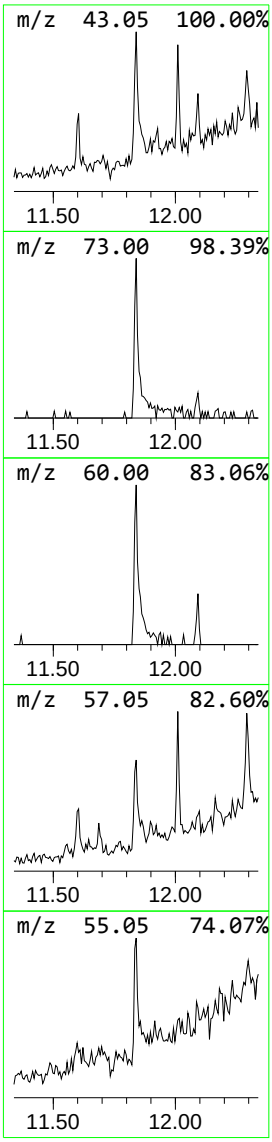
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	2.29 ng	59657	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

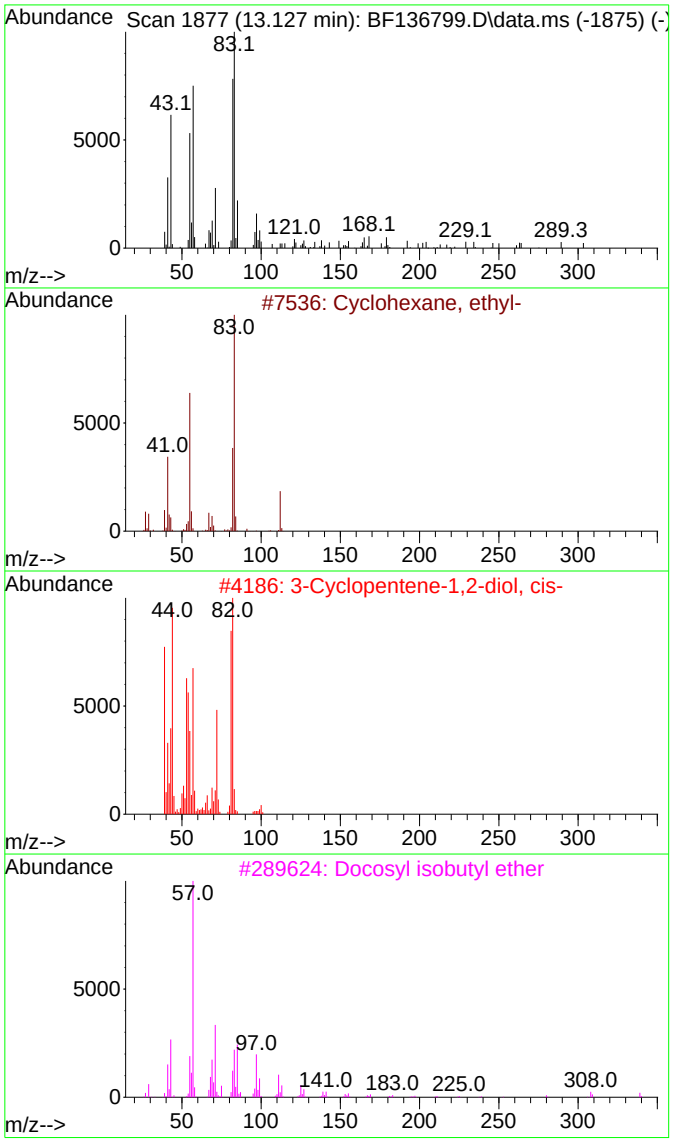
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

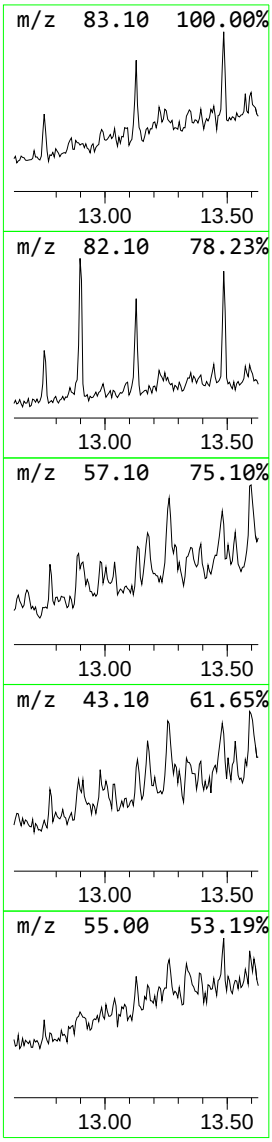
****

Peak Number 4 unknown13.127 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.127	2.32 ng	46082	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, ethyl-	112	C8H16	001678-91-7	27
2	3-Cyclopentene-1,2-diol, cis-	100	C5H8O2	000694-29-1	27
3	Docosyl isobutyl ether	382	C26H54O	1000406-33-1	22
4	Isobutyl tetratriacontyl ether	551	C38H78O	1000406-33-7	22
5	Isobutyl octacosyl ether	467	C32H66O	1000406-33-4	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

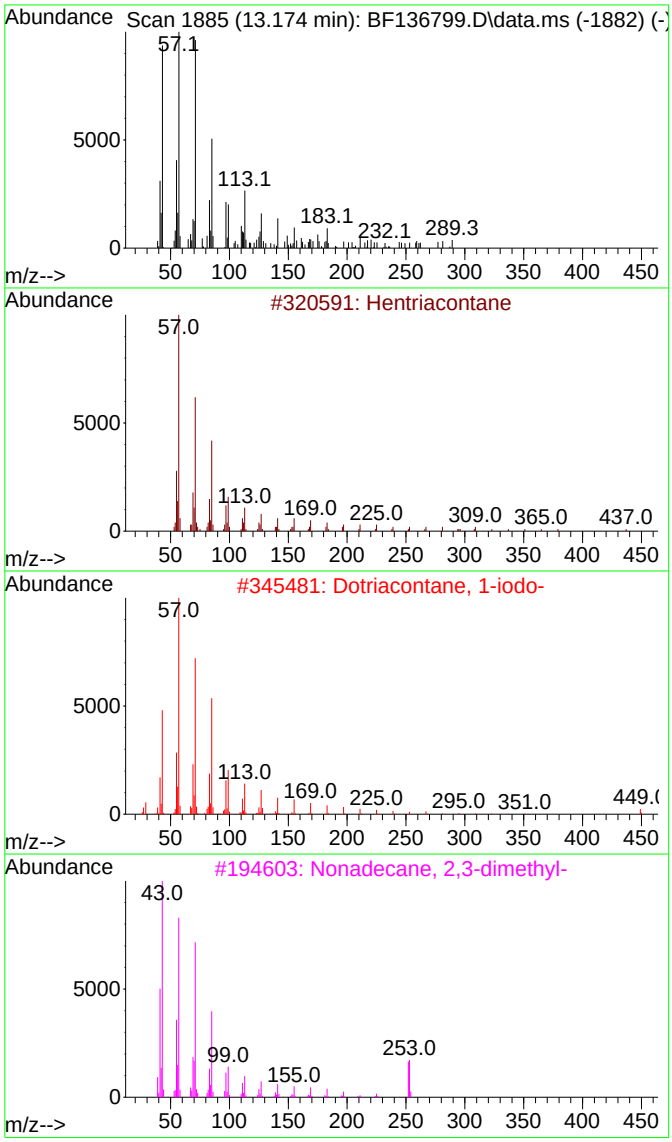
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

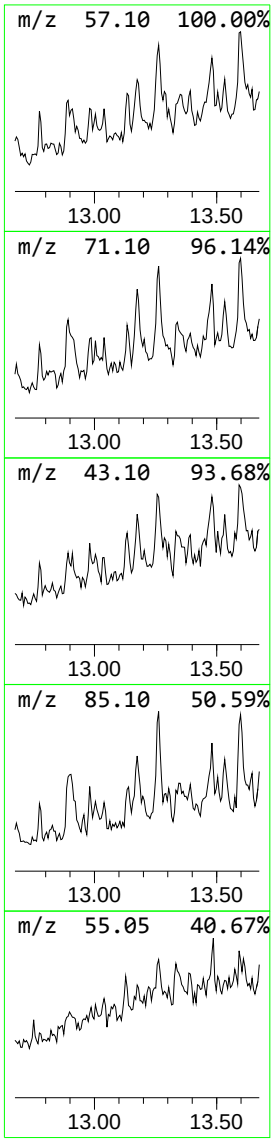
****

Peak Number 5 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.174	3.91 ng	77608	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	83
2	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	83
3	Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	80
4	Triacontane	422	C30H62	000638-68-6	74
5	Tetratetracontane	619	C44H90	007098-22-8	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

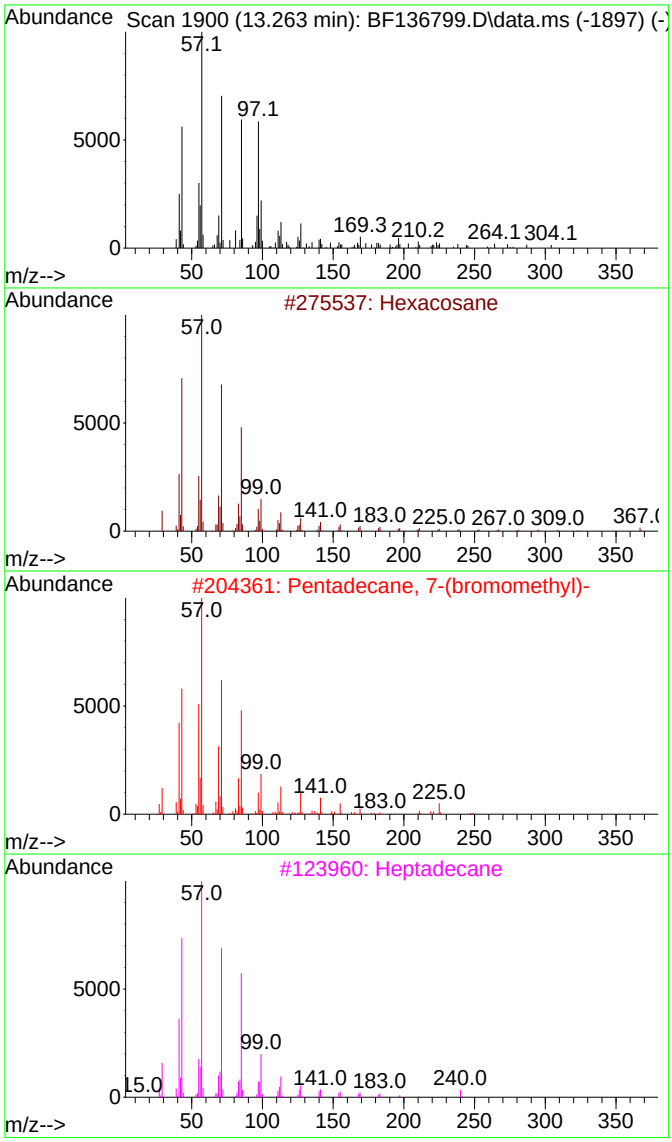
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

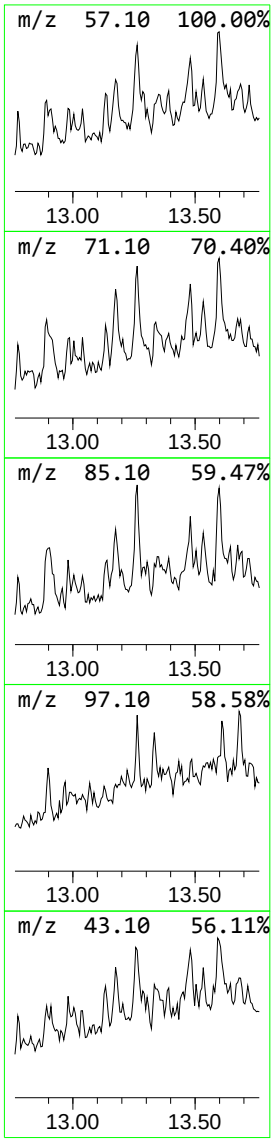
****

Peak Number 6 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.263	3.20 ng	63601	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	72
2	Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	72
3	Heptadecane	240	C17H36	000629-78-7	68
4	Pentacosane	352	C25H52	000629-99-2	64
5	Heneicosane	296	C21H44	000629-94-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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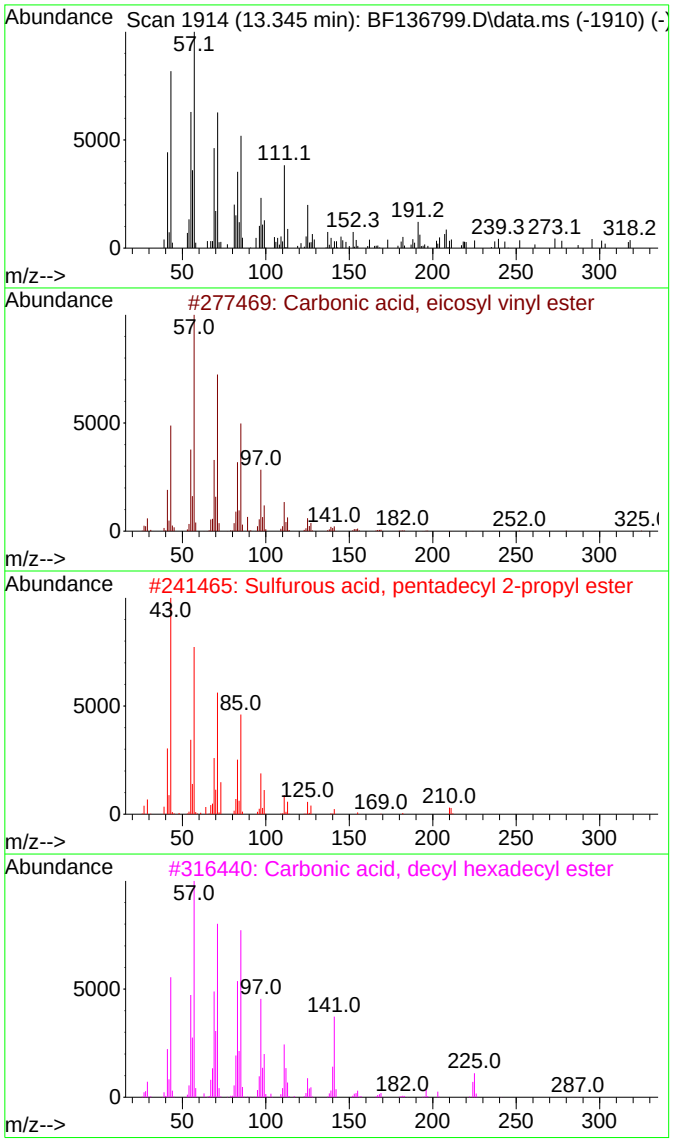
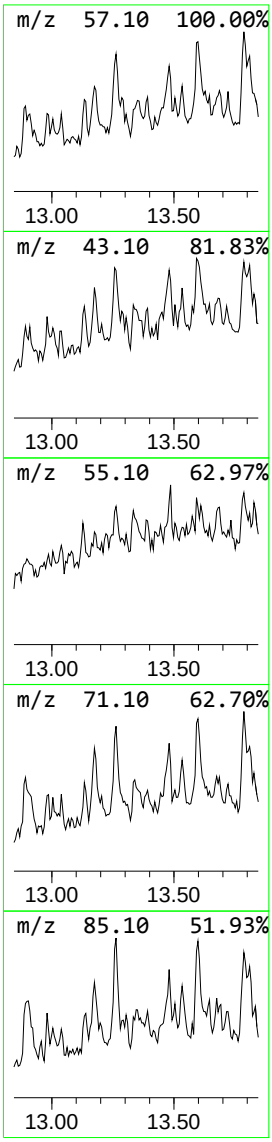
Peak Number 7 unknown13.345 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.345	5.49 ng	109058	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	49
2	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	49
3	Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	49
4	Carbonic acid, decyl tridecyl ester	384	C24H48O3	1000383-16-2	49
5	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1010309-70-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

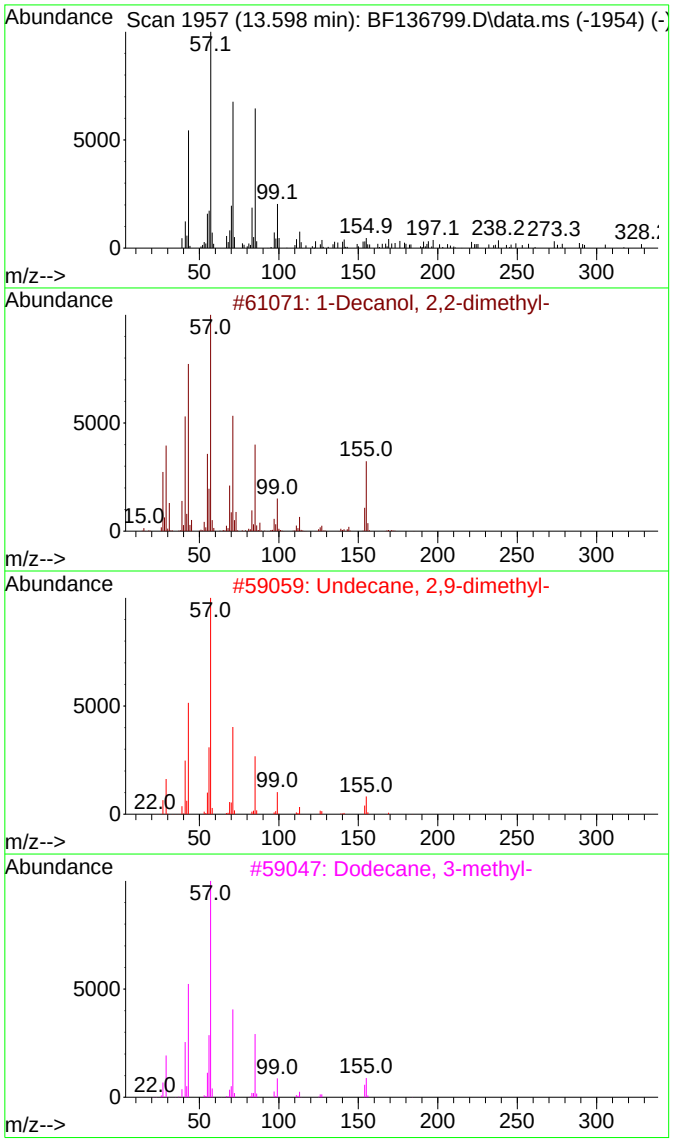
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

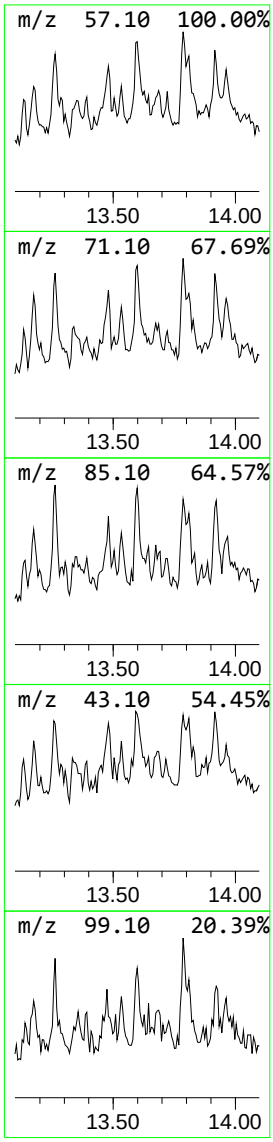
****

Peak Number 8 1-Decanol, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.598	5.42 ng	107601	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2,2-dimethyl-	186	C12H26O	002370-15-2	59
2	Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	53
3	Dodecane, 3-methyl-	184	C13H28	017312-57-1	50
4	Heneicosane	296	C21H44	000629-94-7	47
5	Heptacosane	380	C27H56	000593-49-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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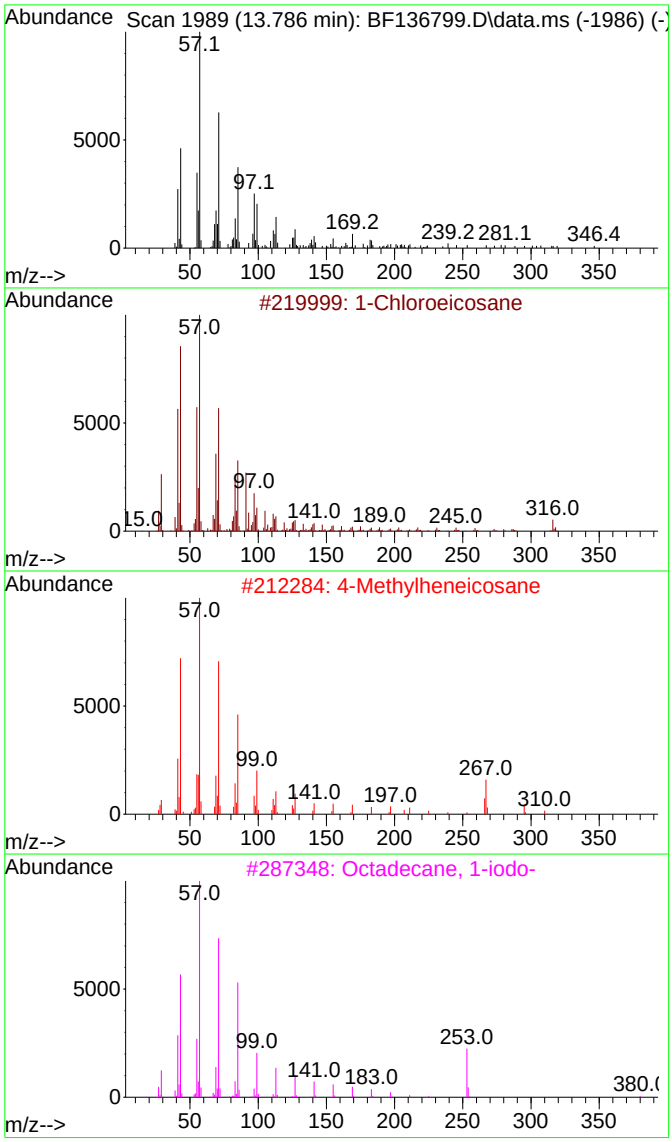
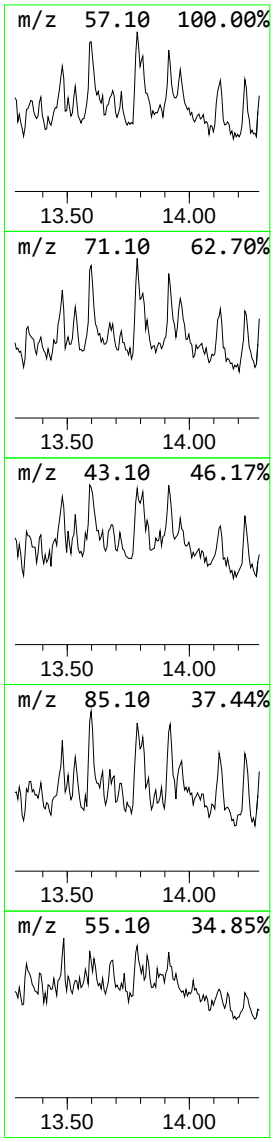
Peak Number 9 1-Chloroeicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.786	5.78 ng	114893	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Chloroeicosane	316	C20H41Cl	042217-02-7	91
2	4-Methylheneicosane	310	C22H46	025117-29-7	74
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	74
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	72
5	Octacosane	394	C28H58	000630-02-4	72





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Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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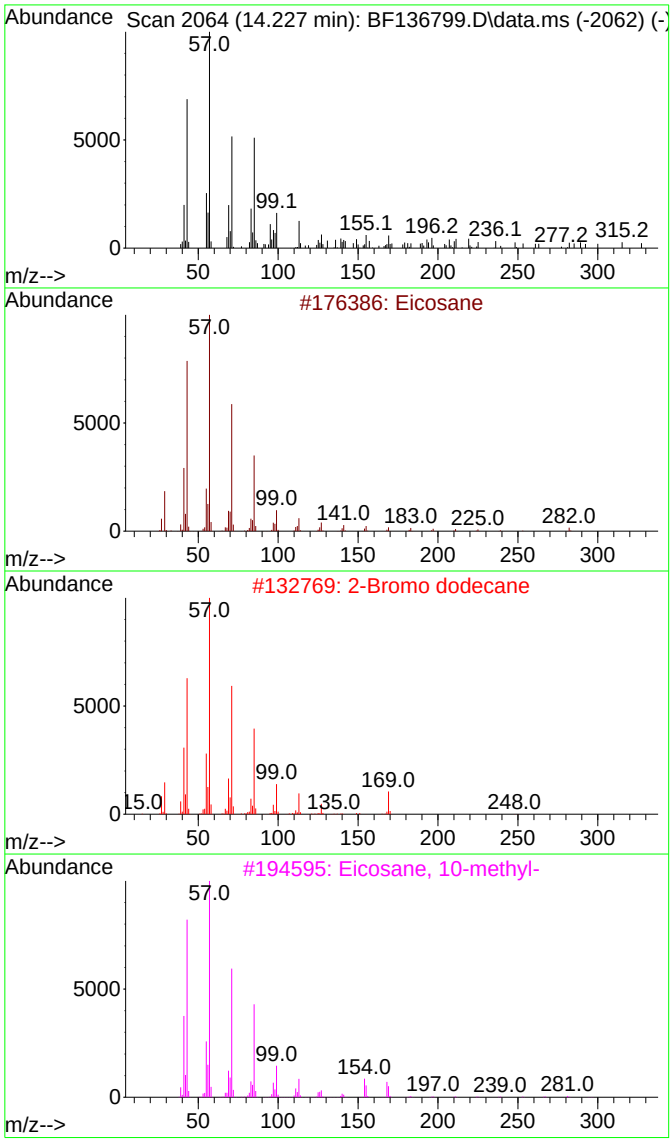
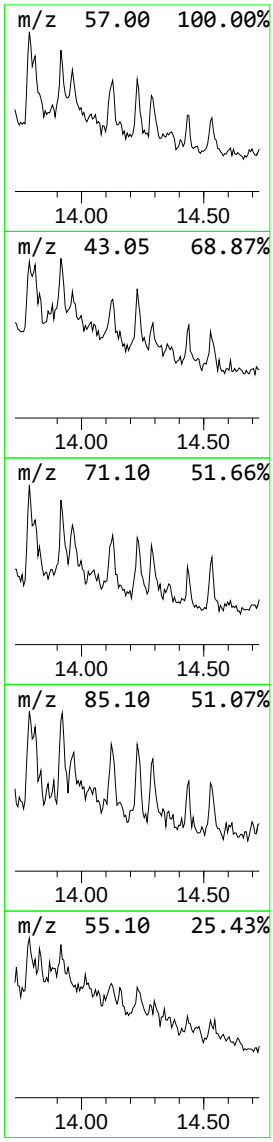
Peak Number 10 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.227	4.09 ng	81297	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	80
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	80
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
4	Octadecane	254	C18H38	000593-45-3	80
5	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	80





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Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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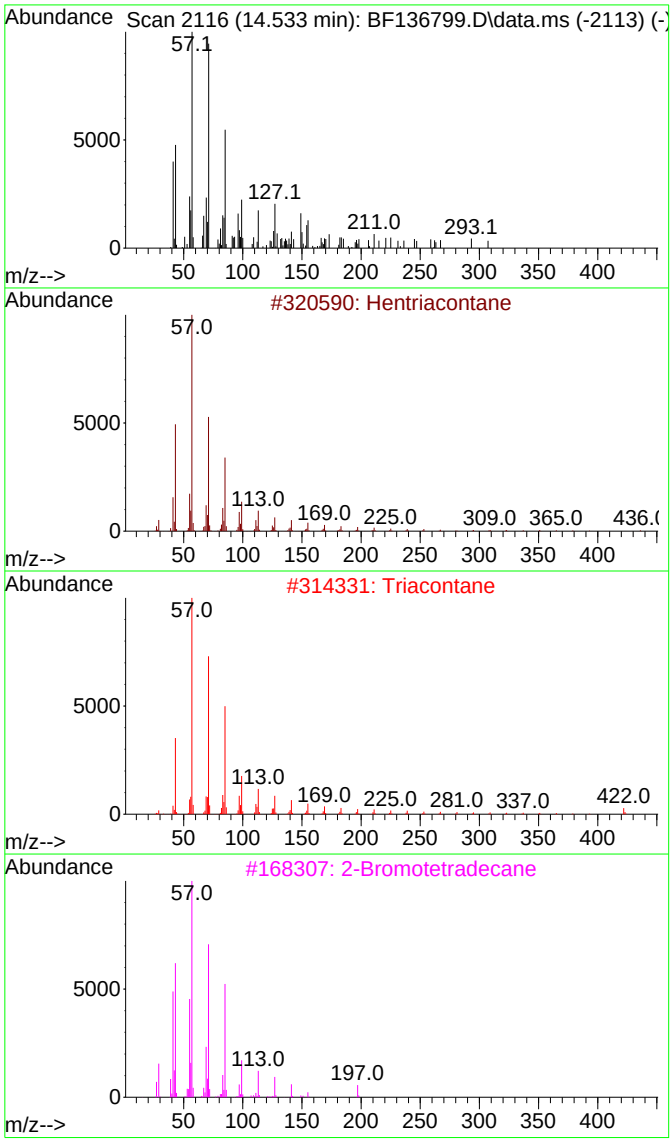
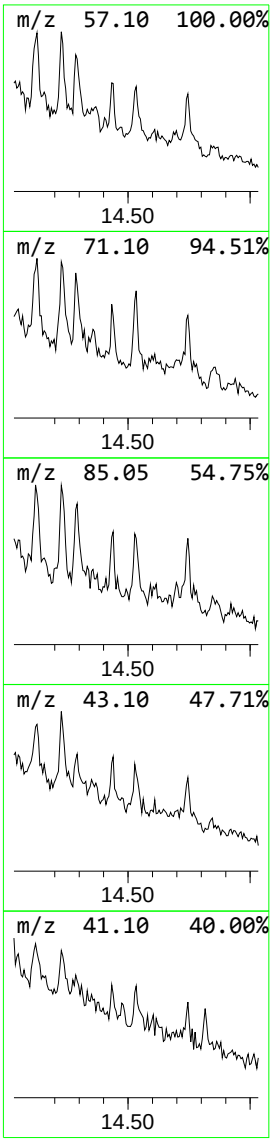
Peak Number 11 Triacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	2.70 ng	53641	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	64
2	Triacontane	422	C30H62	000638-68-6	59
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	59
4	Octacosane	394	C28H58	000630-02-4	59
5	Heneicosane	296	C21H44	000629-94-7	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136799.D
Acq On : 28 Dec 2023 18:16
Operator : CG\JU
Sample : 06027-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIERS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
3-Penten-2-one,...	4.387	4.6	ng	87776	1	6.781	384549	20.0
2-Pentanone, 4-...	5.022	62.5	ng	1201990	1	6.781	384549	20.0
n-Hexadecanoic ...	11.839	2.3	ng	59657	4	11.304	521027	20.0
unknown13.127	13.127	2.3	ng	46082	5	13.963	397309	20.0
Hentriacontane	13.174	3.9	ng	77608	5	13.963	397309	20.0
Hexacosane	13.263	3.2	ng	63601	5	13.963	397309	20.0
unknown13.345	13.345	5.5	ng	109058	5	13.963	397309	20.0
1-Decanol, 2,2-...	13.598	5.4	ng	107601	5	13.963	397309	20.0
1-Chloroeicosane	13.786	5.8	ng	114893	5	13.963	397309	20.0
Eicosane	14.227	4.1	ng	81297	5	13.963	397309	20.0
Triacontane	14.533	2.7	ng	53641	5	13.963	397309	20.0