LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
Data File : BF138623.D
Acq On : 23 Jul 2024 17:33
Operator : RC/JU
Sample : P3248-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-120-SB01

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138623.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	5	12	29	rVB	1290385	2035284	100.00%	14.609%
2	3.387	214	220	235	rBV	51142	113558	5.58%	0.815%
3	5.075	502	507	521	rVB	84094	123550	6.07%	0.887%
4	5.481	570	576	581	rBV	1238546	1591602	78.20%	11.424%
5	6.487	741	747	752	rBV	1281987	1700564	83.55%	12.206%
6	6.681	773	780	791	rBV	18942	27531	1.35%	0.198%
7	6.851	804	809	814	rBV	358707	436348	21.44%	3.132%
8	7.410	898	904	910	rBV	776605	1059088	52.04%	7.602%
9	8.133	1021	1027	1032	rBV	464150	586153	28.80%	4.207%
10	8.445	1075	1080	1085	rBV	38466	55405	2.72%	0.398%
11	9.204	1203	1209	1214	rBV	1440806	1840298	90.42%	13.209%
12	9.886	1319	1325	1330	rBV	526203	658235	32.34%	4.725%
13	9.980	1334	1341	1348	rBV	44293	68954	3.39%	0.495%
14	10.674	1453	1459	1474	rBV	838065	1075053	52.82%	7.717%
15	11.369	1572	1577	1582	rBV	484998	599083	29.43%	4.300%
16	11.892	1661	1666	1681	rBV2	34675	64642	3.18%	0.464%
17	12.951	1841	1846	1851	rBV	938315	1147863	56.40%	8.239%
18	13.863	1995	2001	2017	rBV3	26091	80786	3.97%	0.580%
19	14.004	2020	2025	2034	rVB	250633	318096	15.63%	2.283%
20	15.468	2268	2274	2286	rBV	228892	349576	17.18%	2.509%

Sum of corrected areas: 13931669

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072324\
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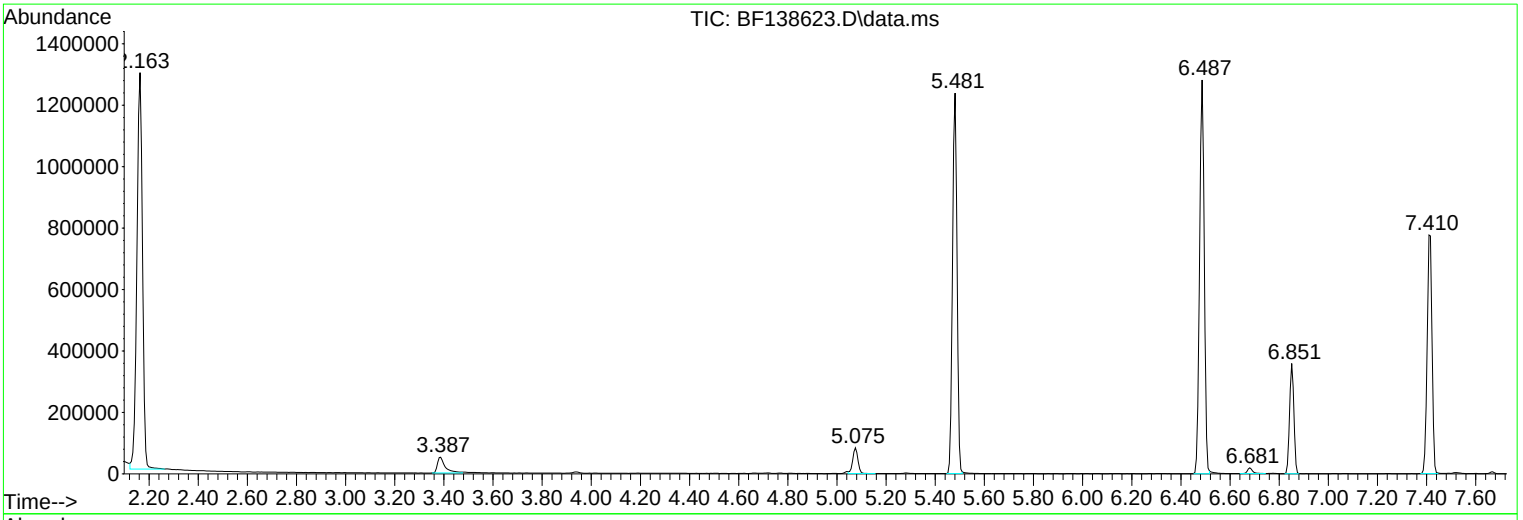
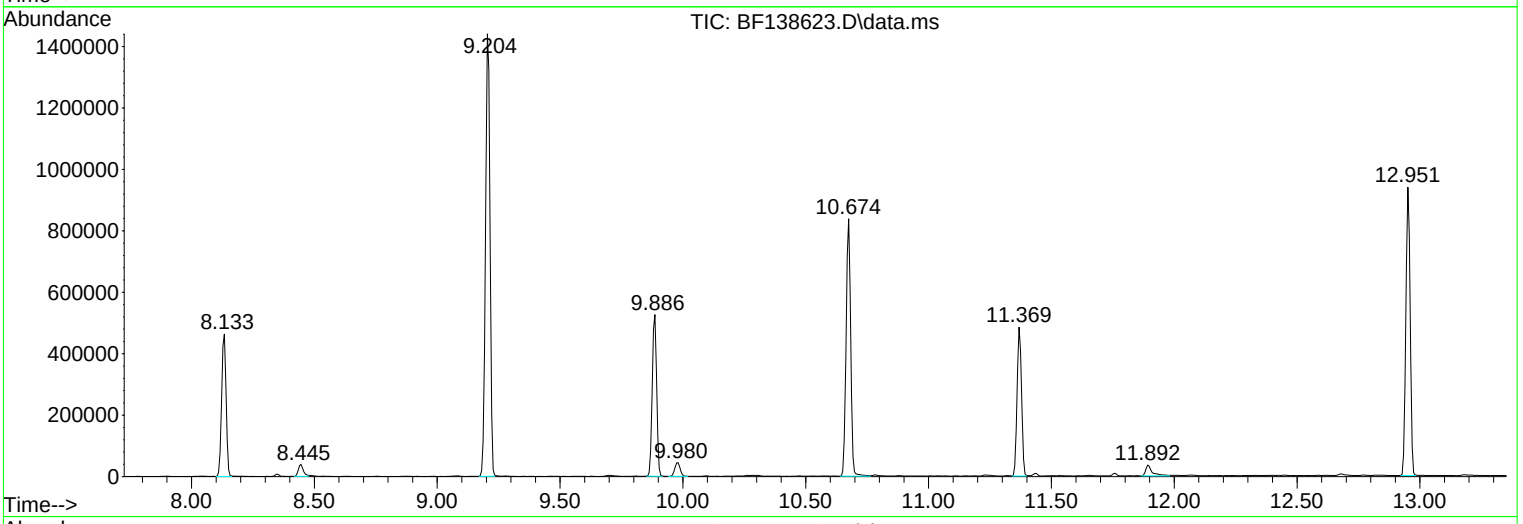
Operator : RC/JU
Sample : P3248-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

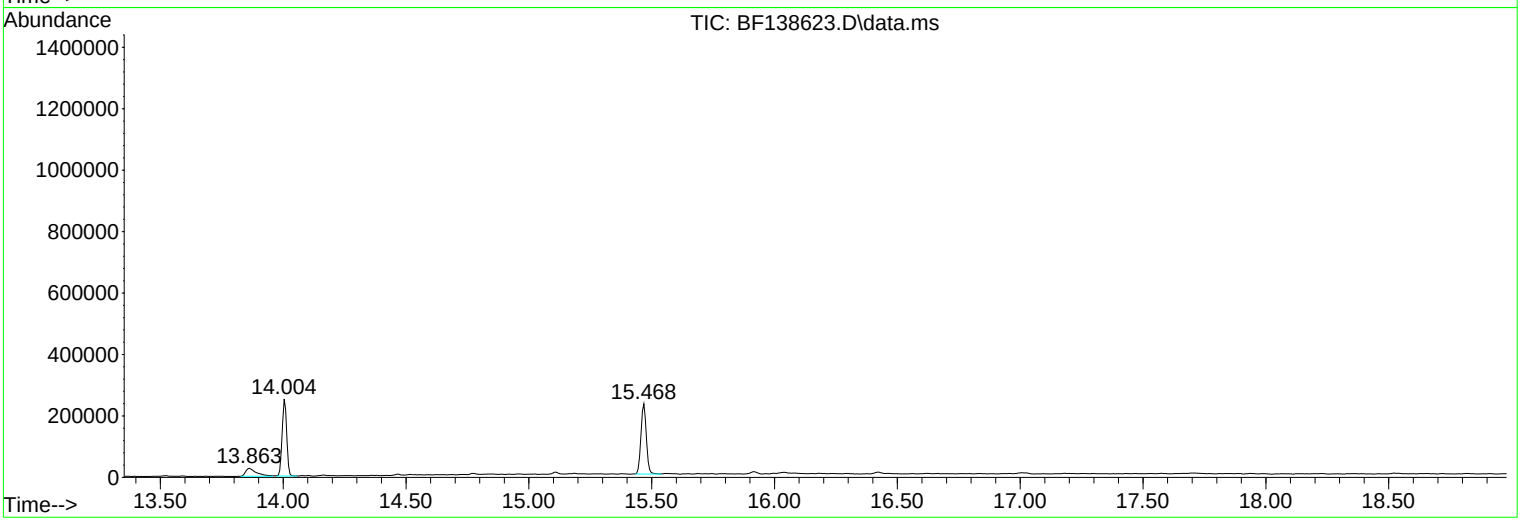
Instrument :
BNA_F
ClientSampleId :
B-120-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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TIC Library : C:\Database\NIST20.L
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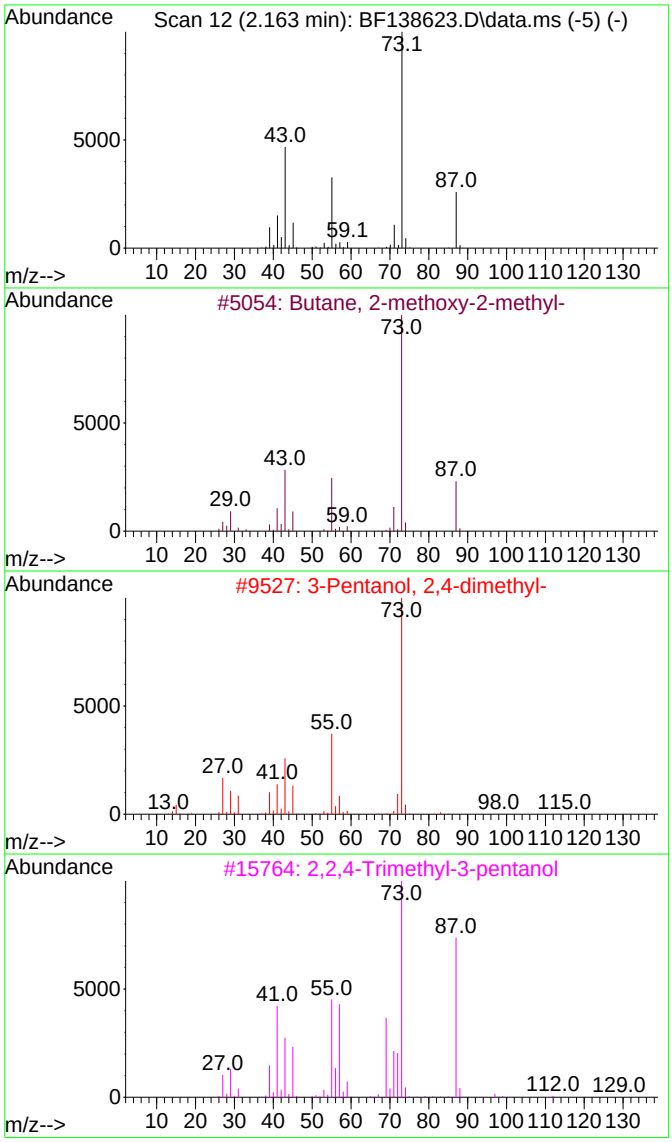
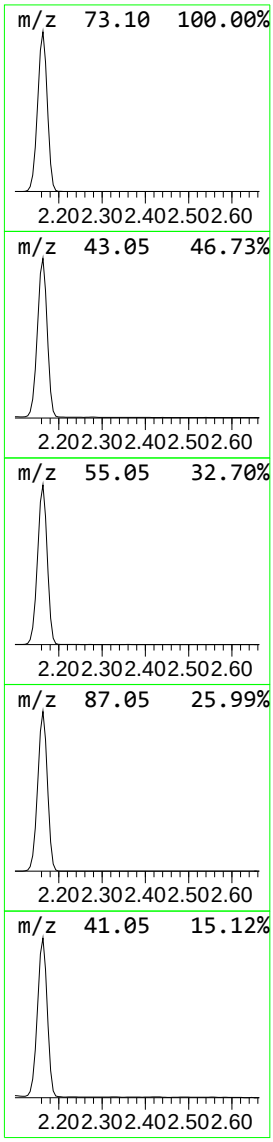
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	93.29 ng	2035280	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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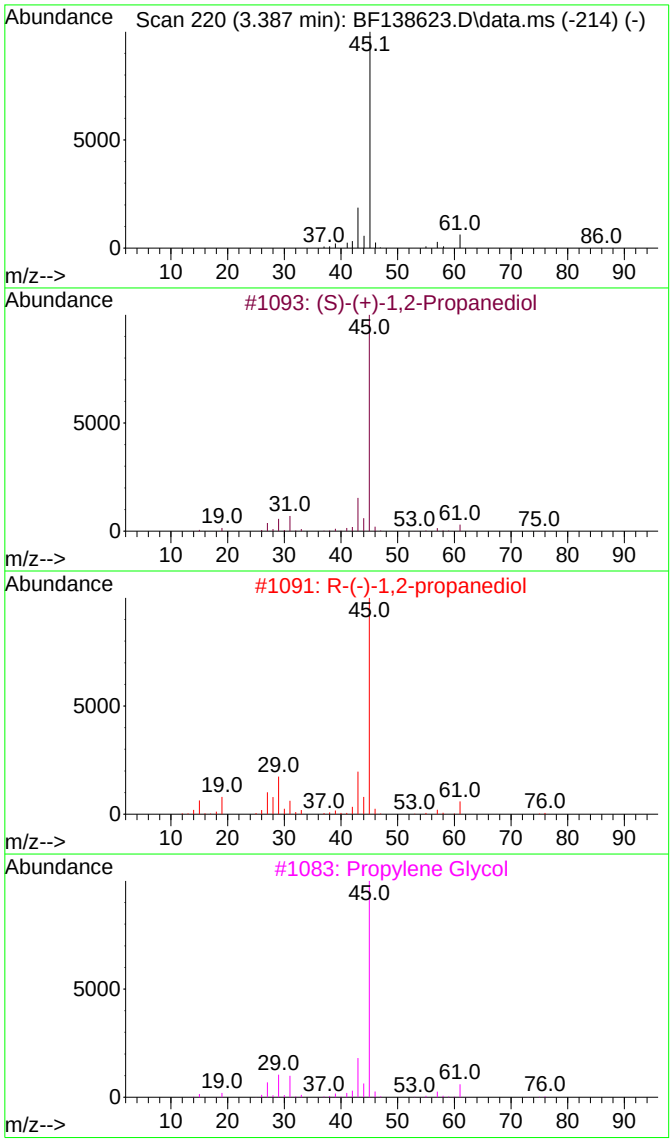
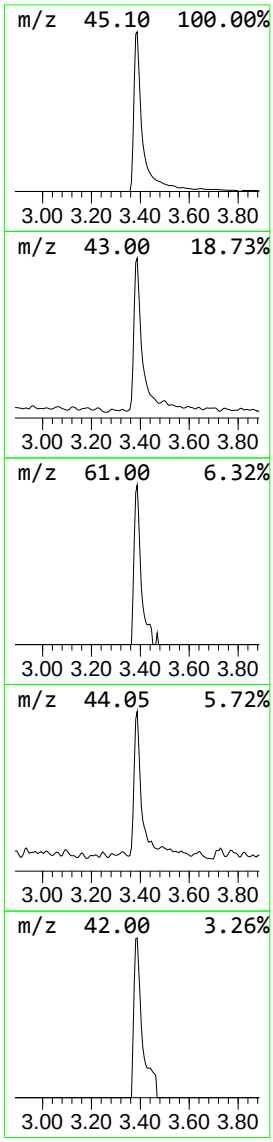
Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	5.20 ng	113558	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	43
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





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Data File : BF138623.D
Acq On : 23 Jul 2024 17:33
Operator : RC/JU
Sample : P3248-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-120-SB01

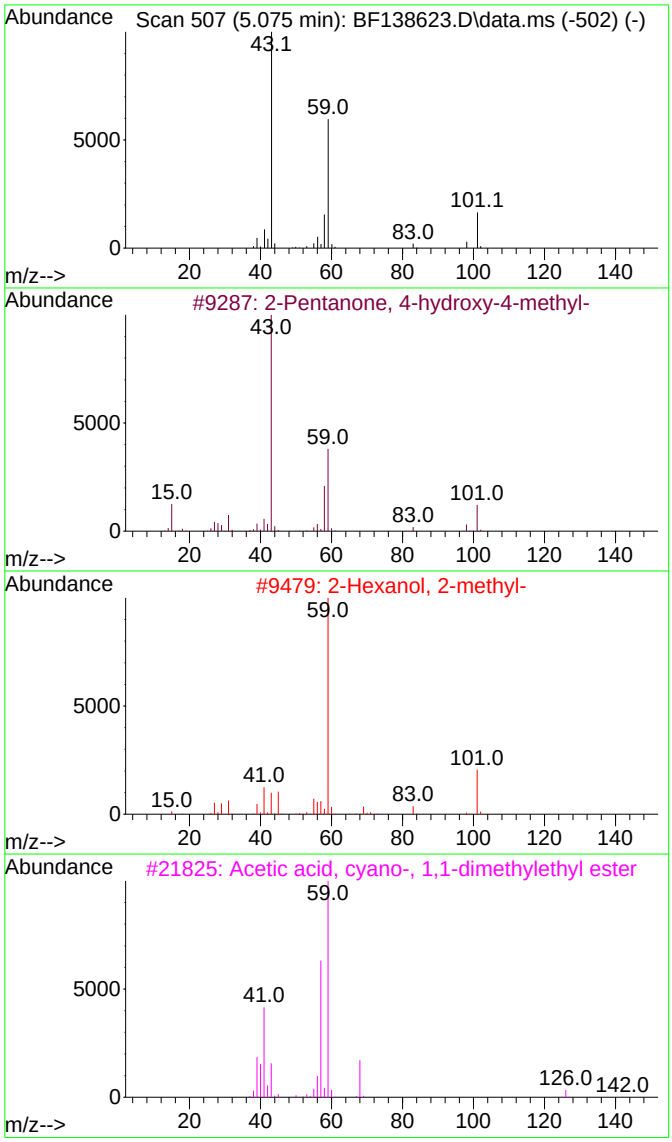
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

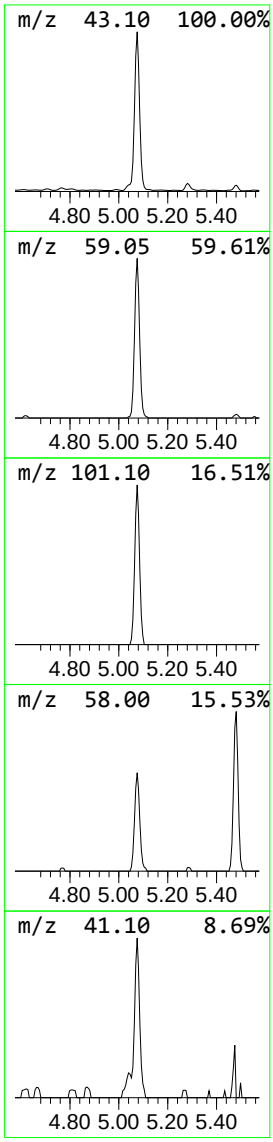
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	5.66 ng	123550	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Sample : P3248-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-120-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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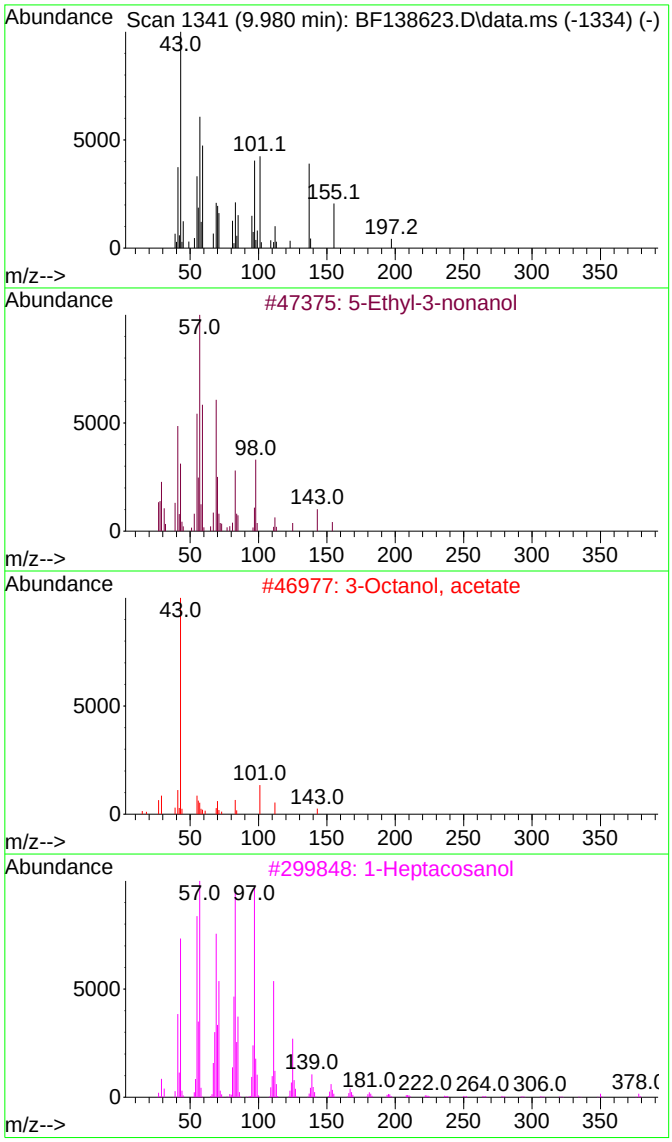
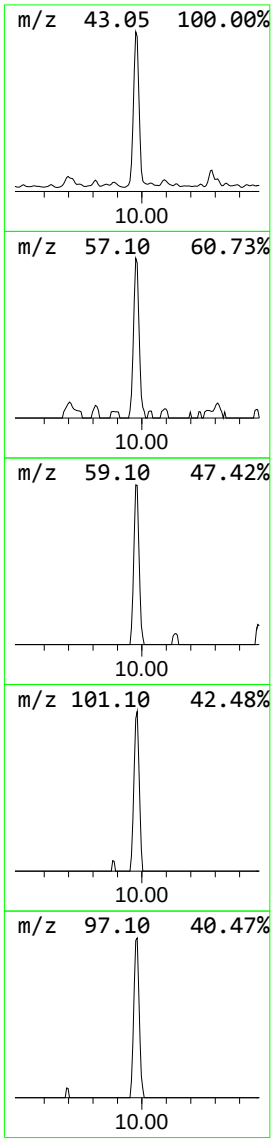
Peak Number 4 unknown9.980 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.980	2.10 ng	68954	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyl-3-nonanol	172	C11H24O	019780-71-3	22
2	3-Octanol, acetate	172	C10H20O2	004864-61-3	22
3	1-Heptacosanol	396	C27H56O	002004-39-9	10
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	10
5	17-Pentatriacontene	491	C35H70	006971-40-0	10





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Data File : BF138623.D
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Operator : RC/JU
Sample : P3248-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-120-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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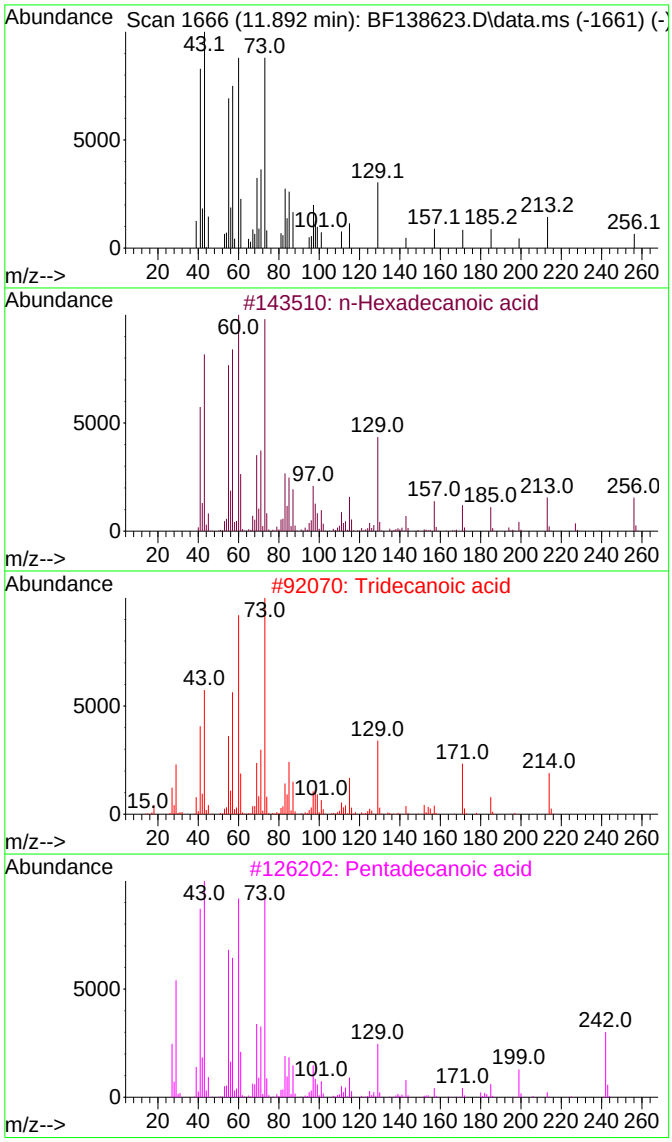
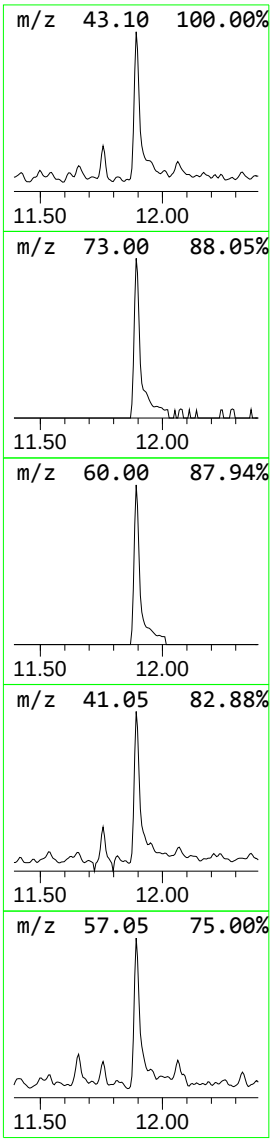
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	2.16 ng	64642	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





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Acq On : 23 Jul 2024 17:33
Operator : RC/JU
Sample : P3248-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-120-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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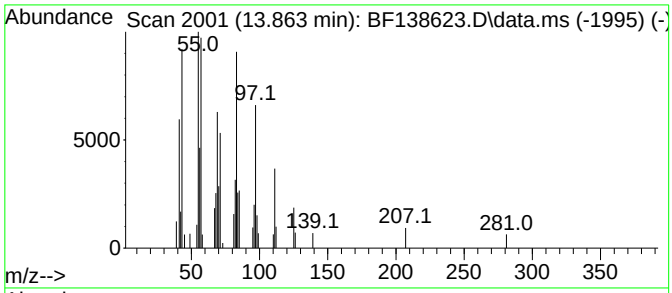
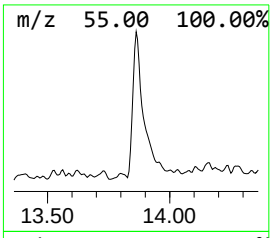
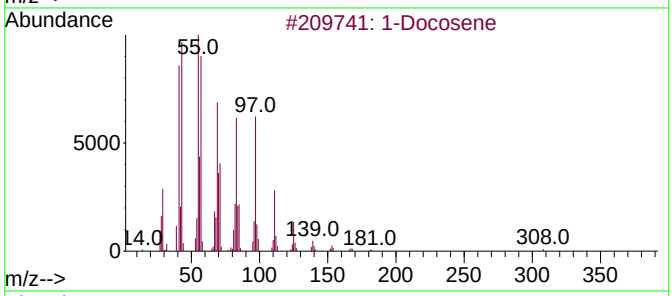
Peak Number 6 1-Docosene Concentration Rank 4

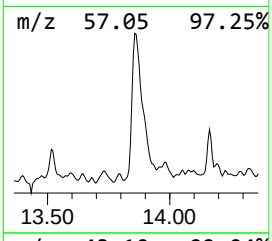
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	5.08 ng	80786	Chrysene-d12	14.004

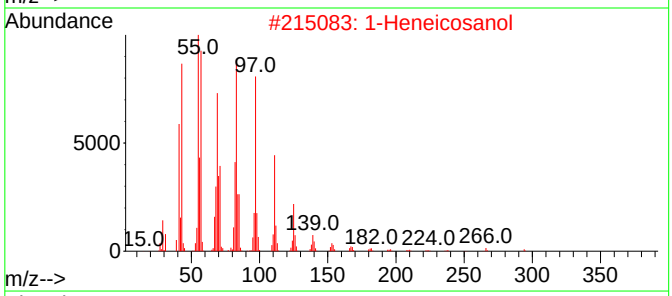
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	Octacosanol	410	C28H58O	000557-61-9	90
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	87

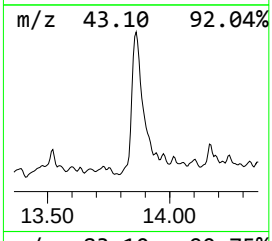


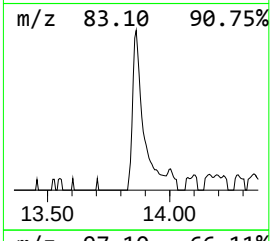


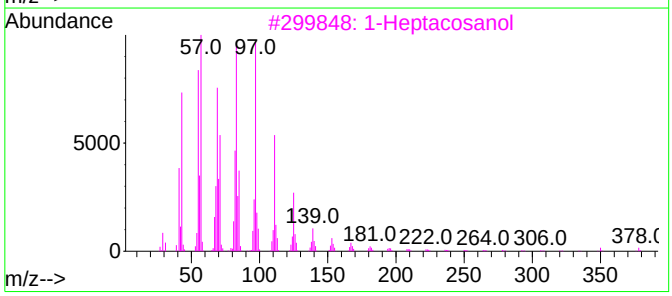


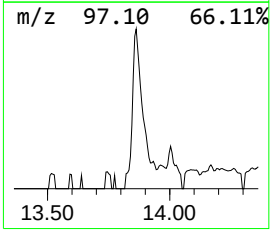












Tentatively Identified Compound (LSC) summary

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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...	2.163	93.3	ng	2035280	1	6.851	436348	20.0
(S)-(+)-1,2-Pro...	3.387	5.2	ng	113558	1	6.851	436348	20.0
2-Pentanone, 4-...	5.075	5.7	ng	123550	1	6.851	436348	20.0
unknown9.980	9.980	2.1	ng	68954	3	9.886	658235	20.0
n-Hexadecanoic ...	11.892	2.2	ng	64642	4	11.369	599083	20.0
1-Docosene	13.863	5.1	ng	80786	5	14.004	318096	20.0