LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136448.D
Acq On : 07 Dec 2023 15:50
Operator : CG\JU
Sample : 05630-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-01-120523

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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136448.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	16	18	23	rVB3	31831	41764	1.86%	0.255%
2	4.334	374	382	386	rVB3	12923	32342	1.44%	0.197%
3	5.040	497	502	506	rBV	223445	257827	11.49%	1.573%
4	5.445	566	571	574	rBV	2183888	1920484	85.55%	11.716%
5	6.445	736	741	744	rBV	2012211	1962584	87.43%	11.973%
6	6.610	765	769	771	rBV	169746	152814	6.81%	0.932%
7	6.634	771	773	777	rVB	154503	119341	5.32%	0.728%
8	6.728	785	789	797	rBV	262740	228376	10.17%	1.393%
9	6.798	797	801	804	rBV	866307	663699	29.57%	4.049%
10	7.357	890	896	899	rBV	1272793	1231401	54.86%	7.512%
11	7.487	905	918	921	rBV	173552	315835	14.07%	1.927%
12	7.616	934	940	946	rVB3	18063	26685	1.19%	0.163%
13	7.816	967	974	981	rBV2	79038	152030	6.77%	0.927%
14	8.075	1012	1018	1021	rBV	1077674	889020	39.60%	5.424%
15	8.486	1085	1088	1092	rBV2	57333	62598	2.79%	0.382%
16	9.157	1197	1202	1205	rBV	2577687	2244785	100.00%	13.695%
17	9.233	1212	1215	1219	rBV2	25393	26161	1.17%	0.160%
18	9.733	1297	1300	1304	rBV	54333	47415	2.11%	0.289%
19	9.833	1313	1317	1320	rBV	1155225	872854	38.88%	5.325%
20	10.622	1448	1451	1455	rBV	1104515	998627	44.49%	6.092%
21	10.757	1469	1474	1480	rVB5	18718	31359	1.40%	0.191%
22	10.951	1501	1507	1511	rBV8	11796	25842	1.15%	0.158%
23	11.069	1523	1527	1535	rVB5	15450	27093	1.21%	0.165%
24	11.322	1567	1570	1573	rBV	783691	673047	29.98%	4.106%
25	11.345	1573	1574	1578	rVB	70774	46012	2.05%	0.281%
26	11.857	1658	1661	1671	rBV	282683	297067	13.23%	1.812%
27	12.539	1774	1777	1781	rBV	73782	75991	3.39%	0.464%
28	12.651	1792	1796	1799	rBV	99496	122637	5.46%	0.748%
29	12.769	1811	1816	1819	rBV	75511	89393	3.98%	0.545%
30	12.921	1838	1842	1845	rBV	1718383	1463029	65.17%	8.926%
31	13.839	1996	1998	2005	rBV3	81819	106407	4.74%	0.649%
32	13.974	2018	2021	2024	rBV	647672	610577	27.20%	3.725%
33	15.462	2270	2274	2281	rVB	459425	576283	25.67%	3.516%

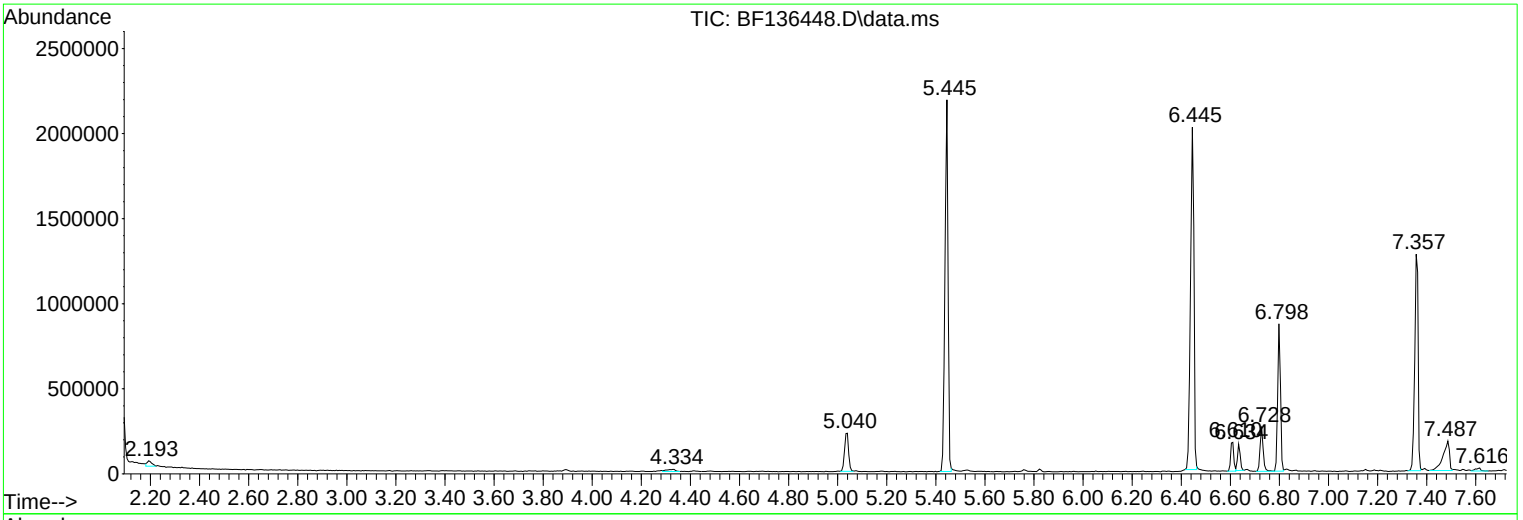
Sum of corrected areas: 16391379

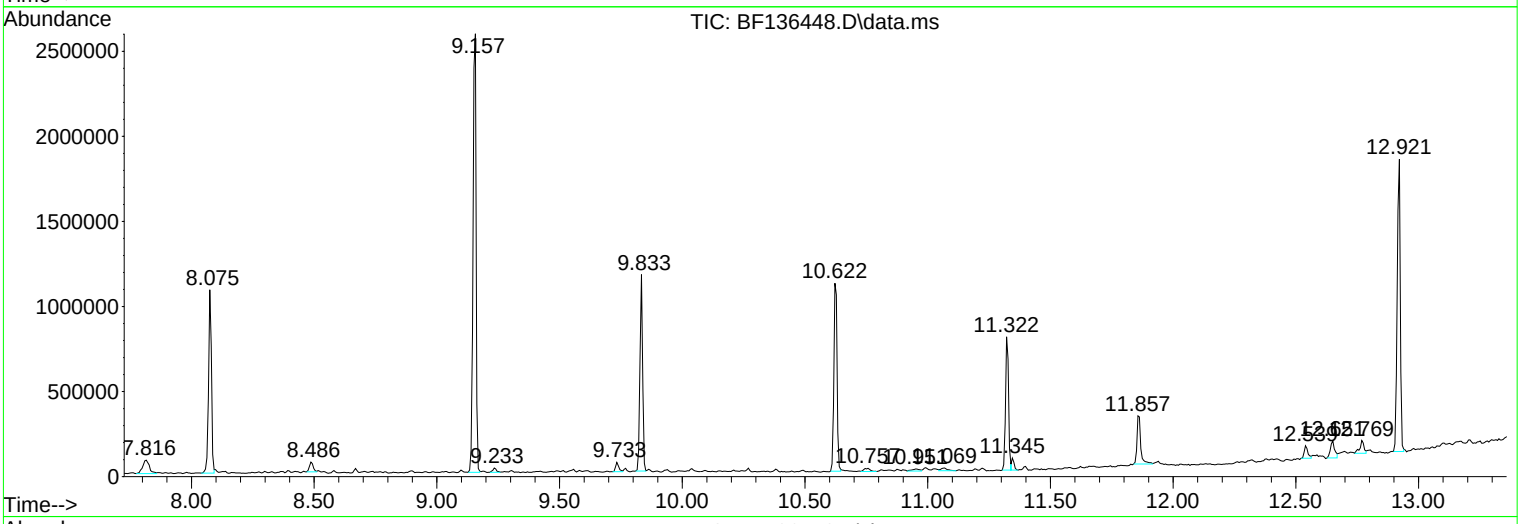
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136448.D
Acq On : 07 Dec 2023 15:50
Operator : CG\JU
Sample : 05630-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

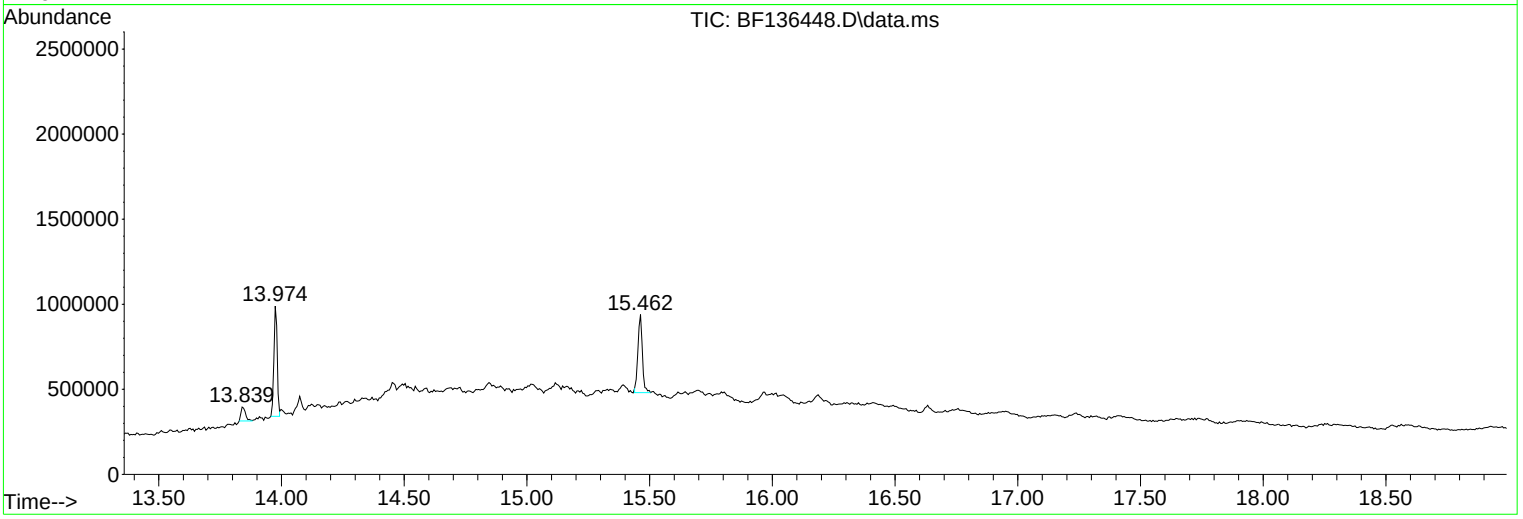
Instrument :
BNA_F
ClientSampleId :
EO-01-120523

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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Data File : BF136448.D
Acq On : 07 Dec 2023 15:50
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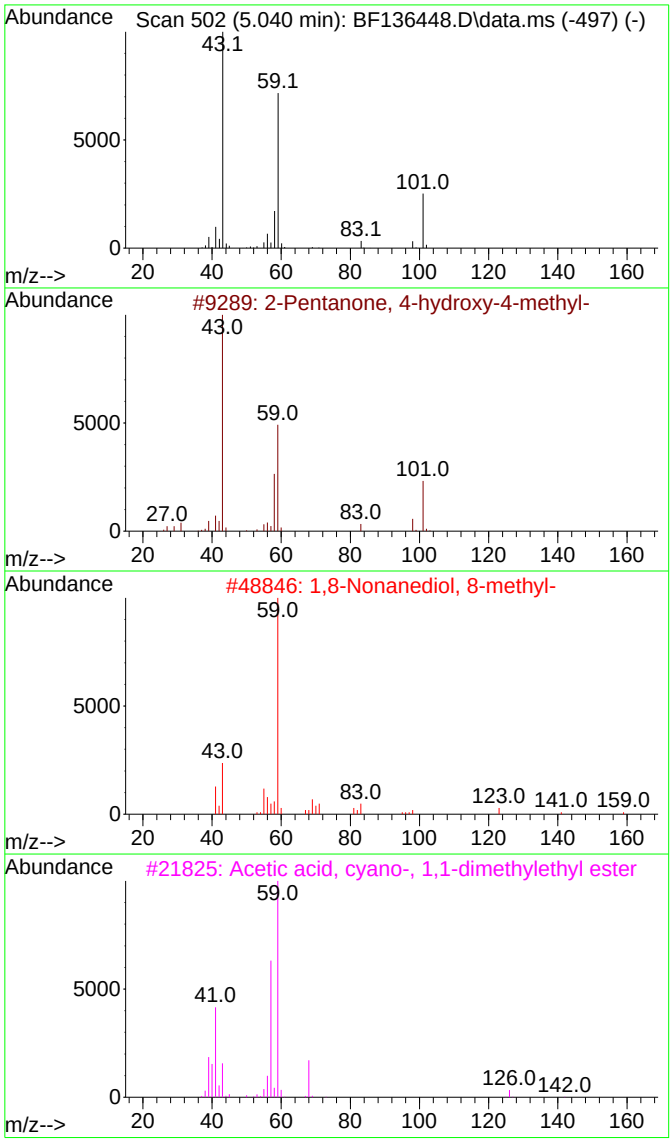
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

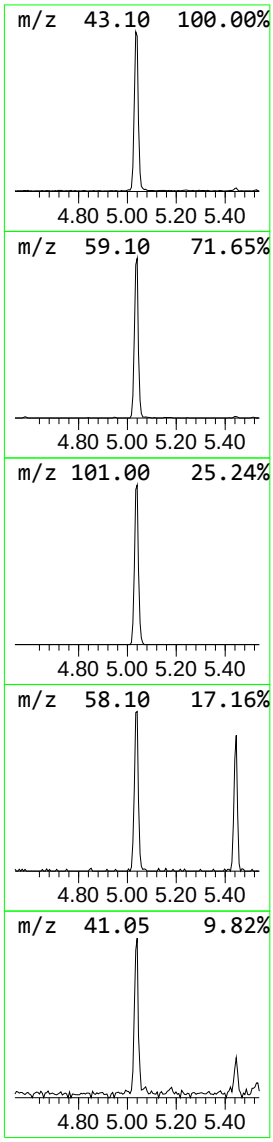
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	7.77 ng	257827	1,4-Dichlorobenzene-d4	6.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Data File : BF136448.D
Acq On : 07 Dec 2023 15:50
Operator : CG\JU
Sample : 05630-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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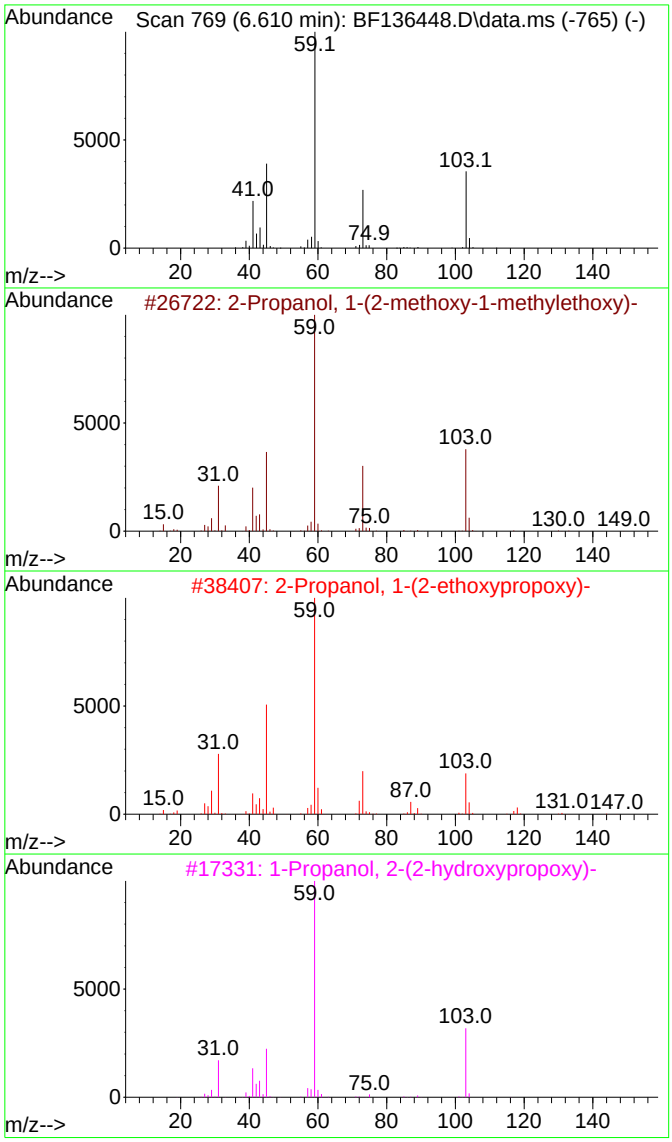
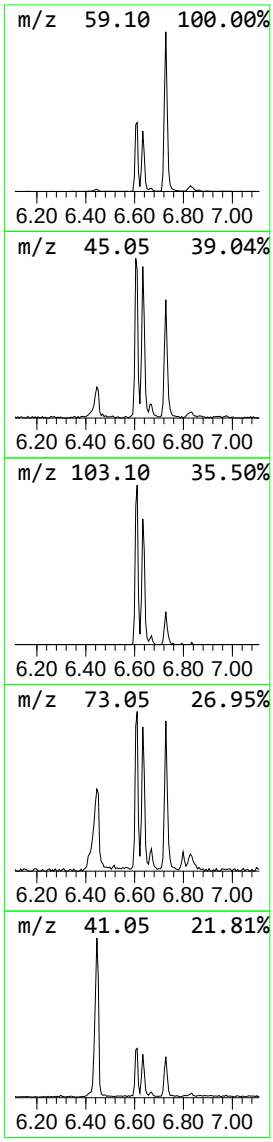
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.610	4.60 ng	152814	1,4-Dichlorobenzene-d4	6.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	90
2	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	72
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	50
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	50





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Acq On : 07 Dec 2023 15:50
Operator : CG\JU
Sample : 05630-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-01-120523

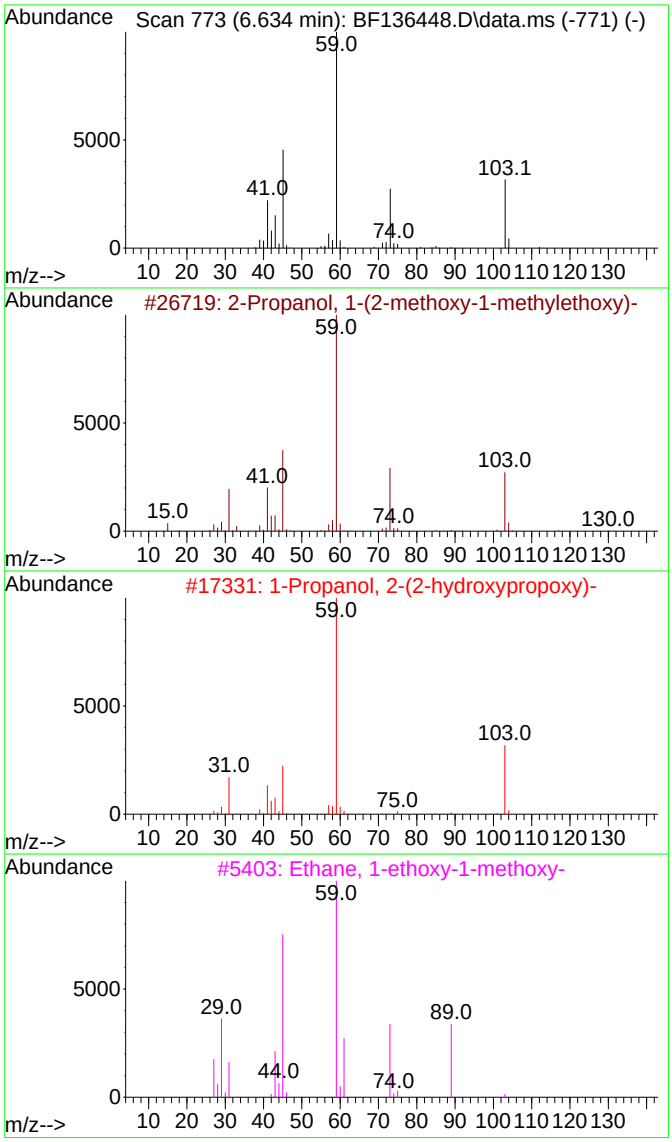
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

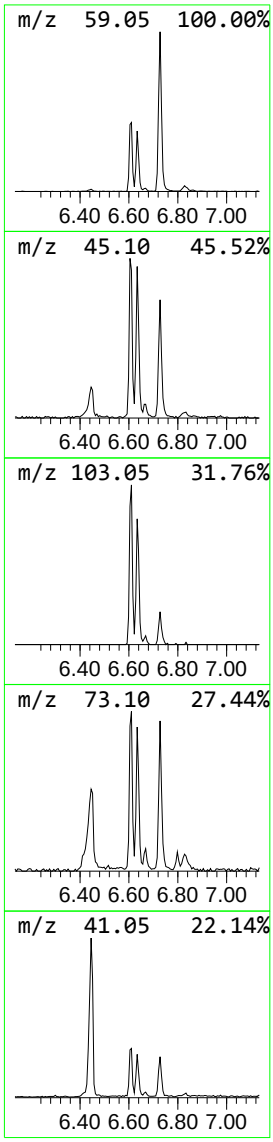
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Propanol, 2-(2-hydroxypro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.634	3.60 ng	119341	1,4-Dichlorobenzene-d4	6.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
3	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	50
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
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Operator : CG\JU
Sample : 05630-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-01-120523

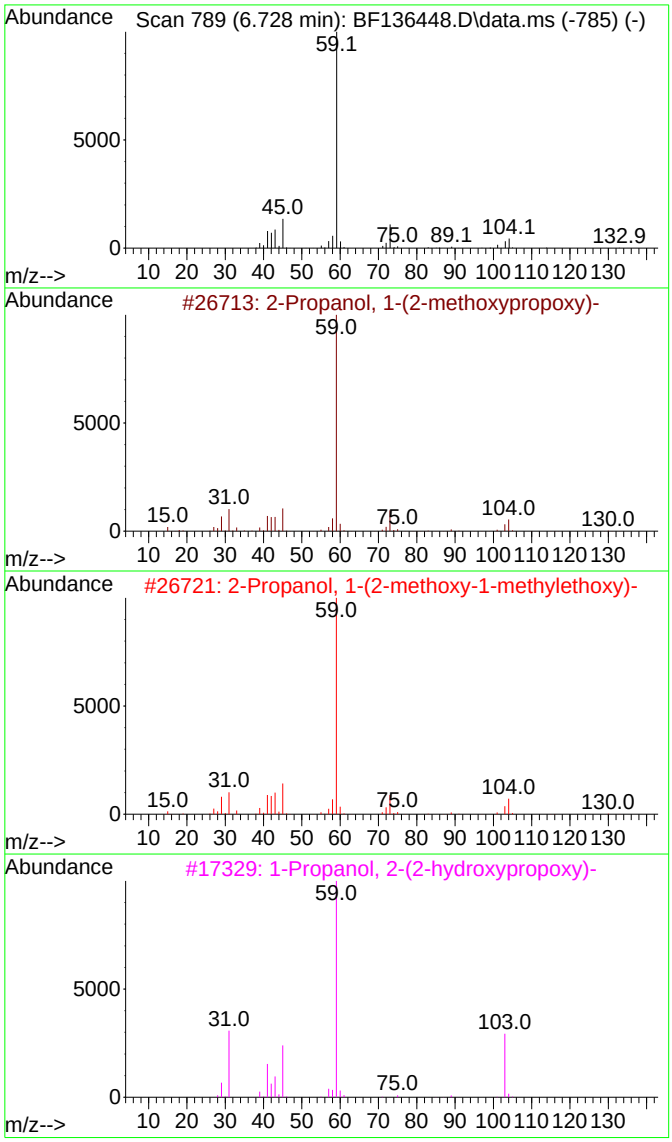
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

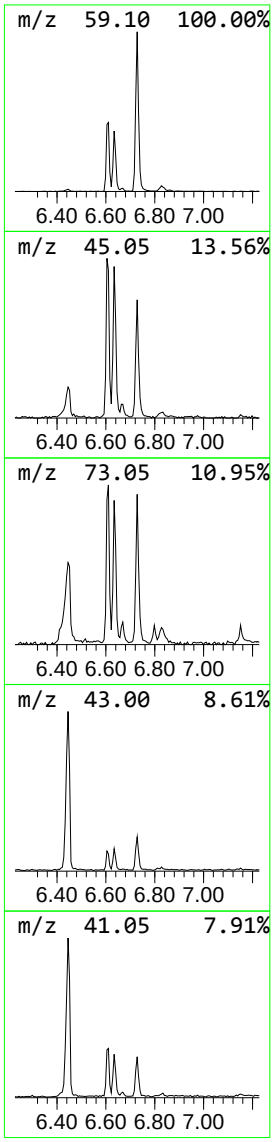
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Propanol, 1-(2-methoxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.728	6.88 ng	228376	1,4-Dichlorobenzene-d4	6.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
4	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	50
5	Tetraglyme	222	C10H22O5	000143-24-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
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Operator : CG\JU
Sample : 05630-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-01-120523

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

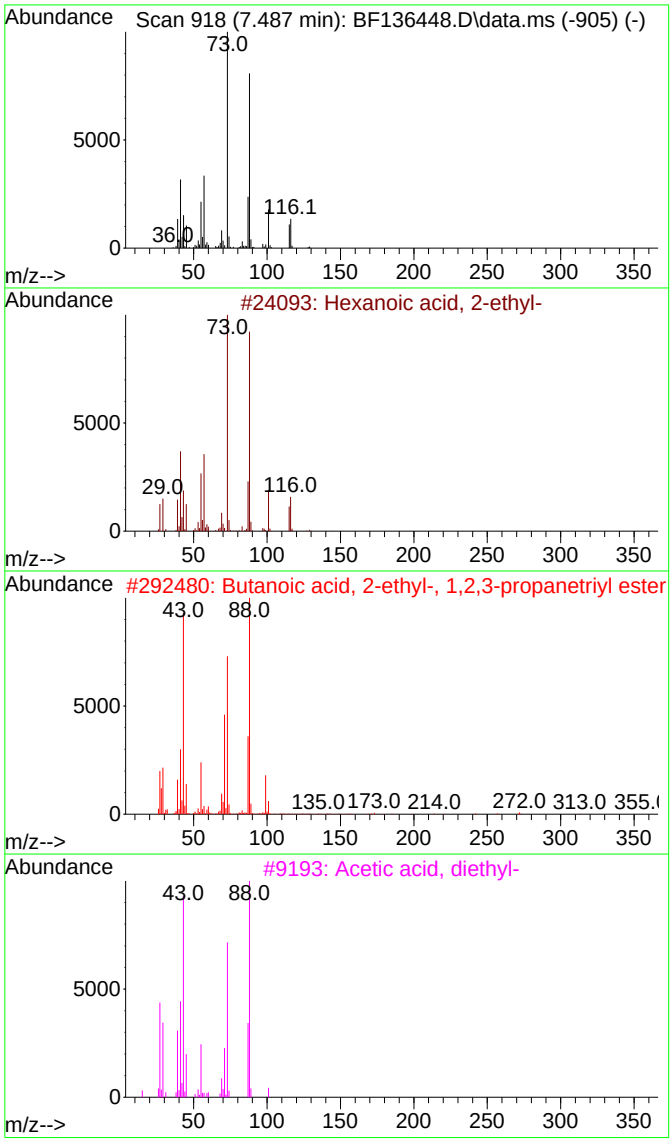
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

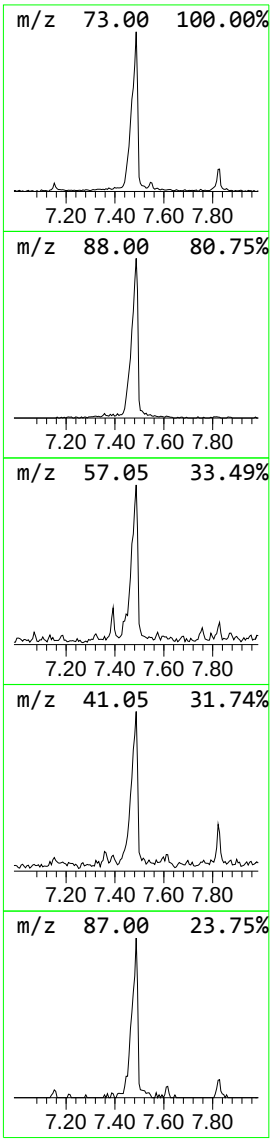
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.487	7.11 ng	315835	Naphthalene-d8	8.075

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	59
4	Heptanoic acid, 2-methyl-, methy...	158	C9H18O2	051209-78-0	47
5	Methyl-2,3,4--tri-O-methyl.alpha...	220	C10H20O5	003253-23-4	42





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Sample : 05630-01
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Instrument :
BNA_F
ClientSampleId :
EO-01-120523

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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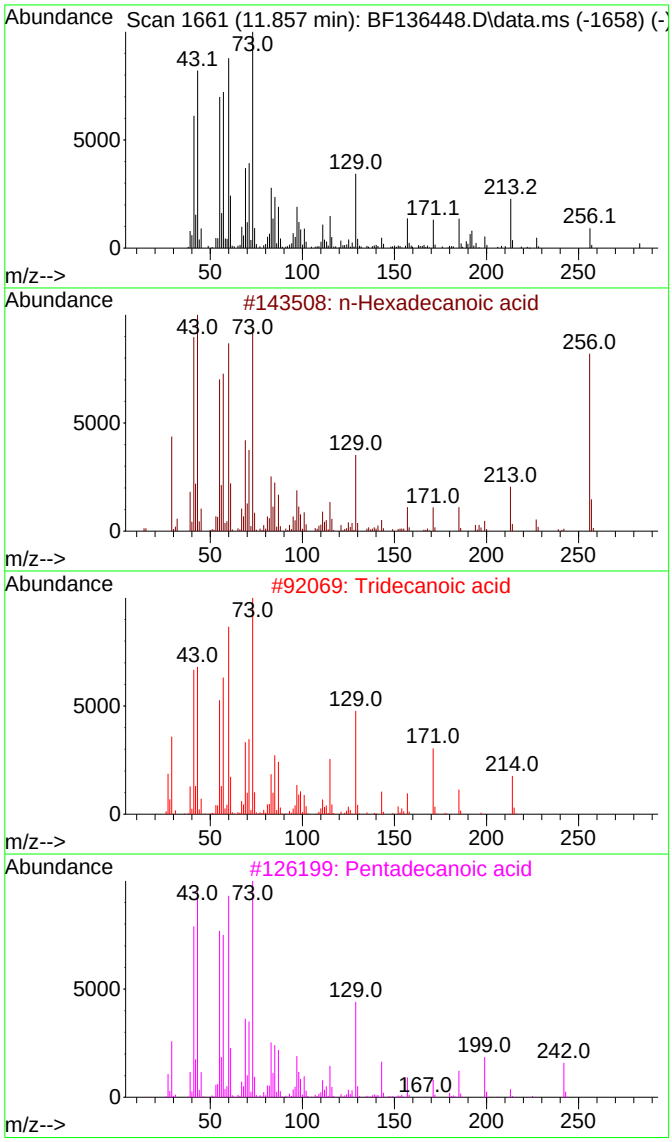
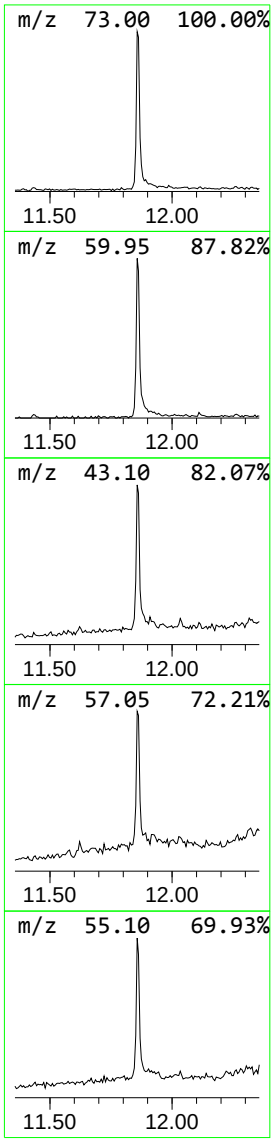
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	8.83 ng	297067	Phenanthrene-d10	11.322

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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Acq On : 07 Dec 2023 15:50
Operator : CG\JU
Sample : 05630-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-01-120523

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

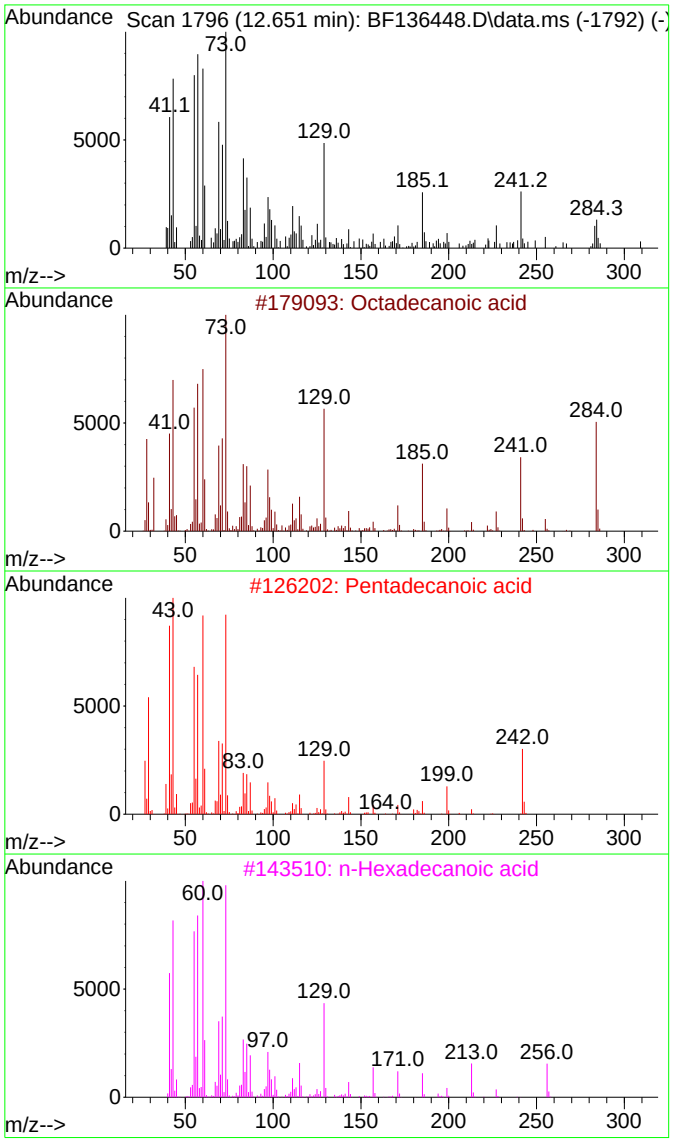
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

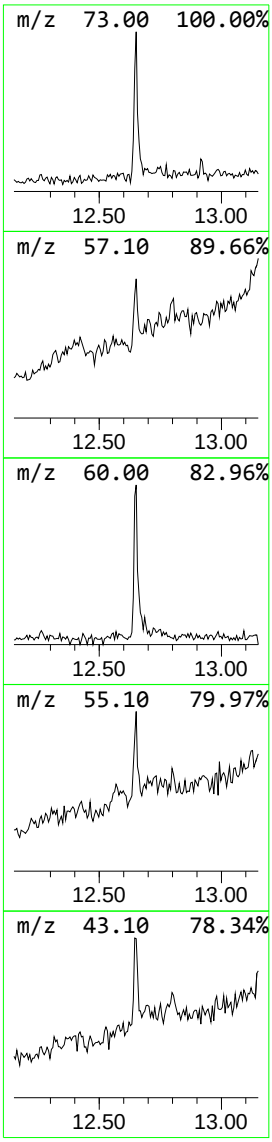
****

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	4.02 ng	122637	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	52





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Instrument :
BNA_F
ClientSampleId :
EO-01-120523

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

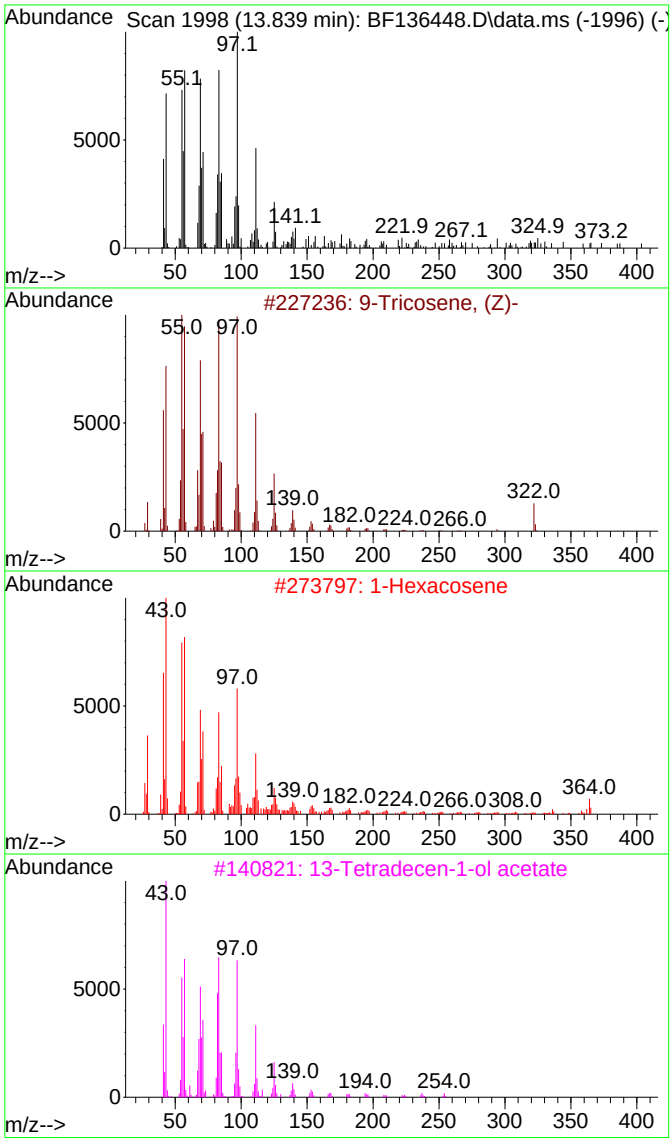
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

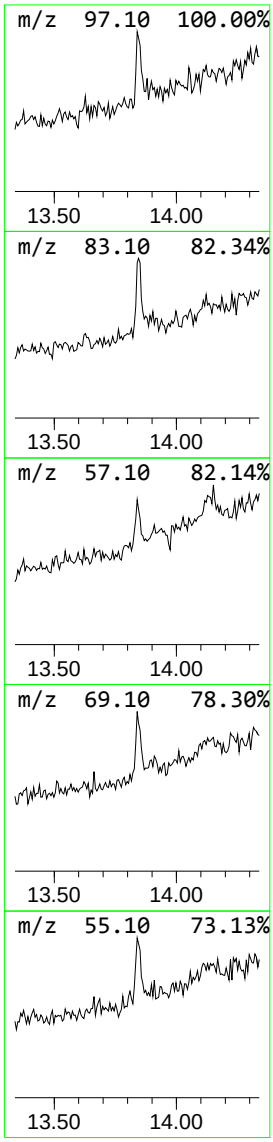
****

Peak Number 10 9-Tricosene, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	3.49 ng	106407	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136448.D
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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-...	5.040	7.8	ng	257827	1	6.798	663699	20.0
2-Propanol, 1-(...	6.610	4.6	ng	152814	1	6.798	663699	20.0
1-Propanol, 2-(...	6.634	3.6	ng	119341	1	6.798	663699	20.0
2-Propanol, 1-(...	6.728	6.9	ng	228376	1	6.798	663699	20.0
Hexanoic acid, ...	7.487	7.1	ng	315835	2	8.075	889020	20.0
n-Hexadecanoic ...	11.857	8.8	ng	297067	4	11.322	673047	20.0
Octadecanoic acid	12.651	4.0	ng	122637	5	13.974	610577	20.0
9-Tricosene, (Z)-	13.839	3.5	ng	106407	5	13.974	610577	20.0