LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102922\
Data File : BM037269.D
Acq On : 29 Oct 2022 14:05
Operator : CG/JU
Sample : N5266-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221099-204-SITE-WATER

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_M\Methods\8270-BM102822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	315	322	329	rVB	489018	692810	3.08%	0.563%
2	5.445	394	401	414	rBV	5354420	7823816	34.74%	6.355%
3	7.045	666	673	689	rBV	4385555	6896333	30.62%	5.602%
4	7.869	806	813	821	rBV	1661735	2594402	11.52%	2.107%
5	9.045	1005	1013	1027	rBV	5907671	9566740	42.48%	7.771%
6	10.457	1245	1253	1263	rBV	214070	420734	1.87%	0.342%
7	10.674	1282	1290	1297	rBV	2091227	3443429	15.29%	2.797%
8	13.133	1700	1708	1723	rBV	15174610	21101045	93.69%	17.140%
9	14.504	1935	1941	1952	rBV	2718392	4039554	17.94%	3.281%
10	15.992	2187	2194	2213	rBV	8846660	12694391	56.36%	10.311%
11	17.245	2401	2407	2418	rBV	2838569	4104695	18.22%	3.334%
12	18.145	2554	2560	2587	rBV	1410361	3154865	14.01%	2.563%
13	19.303	2748	2757	2772	rBV	1727666	4858689	21.57%	3.947%
14	19.415	2772	2776	2795	rVB	3102023	5395818	23.96%	4.383%
15	19.868	2847	2853	2858	rBV	19472304	22523042	100.00%	18.295%
16	20.180	2902	2906	2913	rVB2	306077	367364	1.63%	0.298%
17	20.821	3011	3015	3023	rVB	546683	658896	2.93%	0.535%
18	21.062	3050	3056	3063	rBV	2177168	3346550	14.86%	2.718%
19	21.127	3064	3067	3070	rVV2	446167	665619	2.96%	0.541%
20	21.162	3070	3073	3084	rVB2	451819	769341	3.42%	0.625%
21	21.415	3112	3116	3126	rBV	3021382	3924939	17.43%	3.188%
22	23.774	3512	3517	3528	rVB2	2017802	4068355	18.06%	3.305%

Sum of corrected areas: 123111427

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102922\
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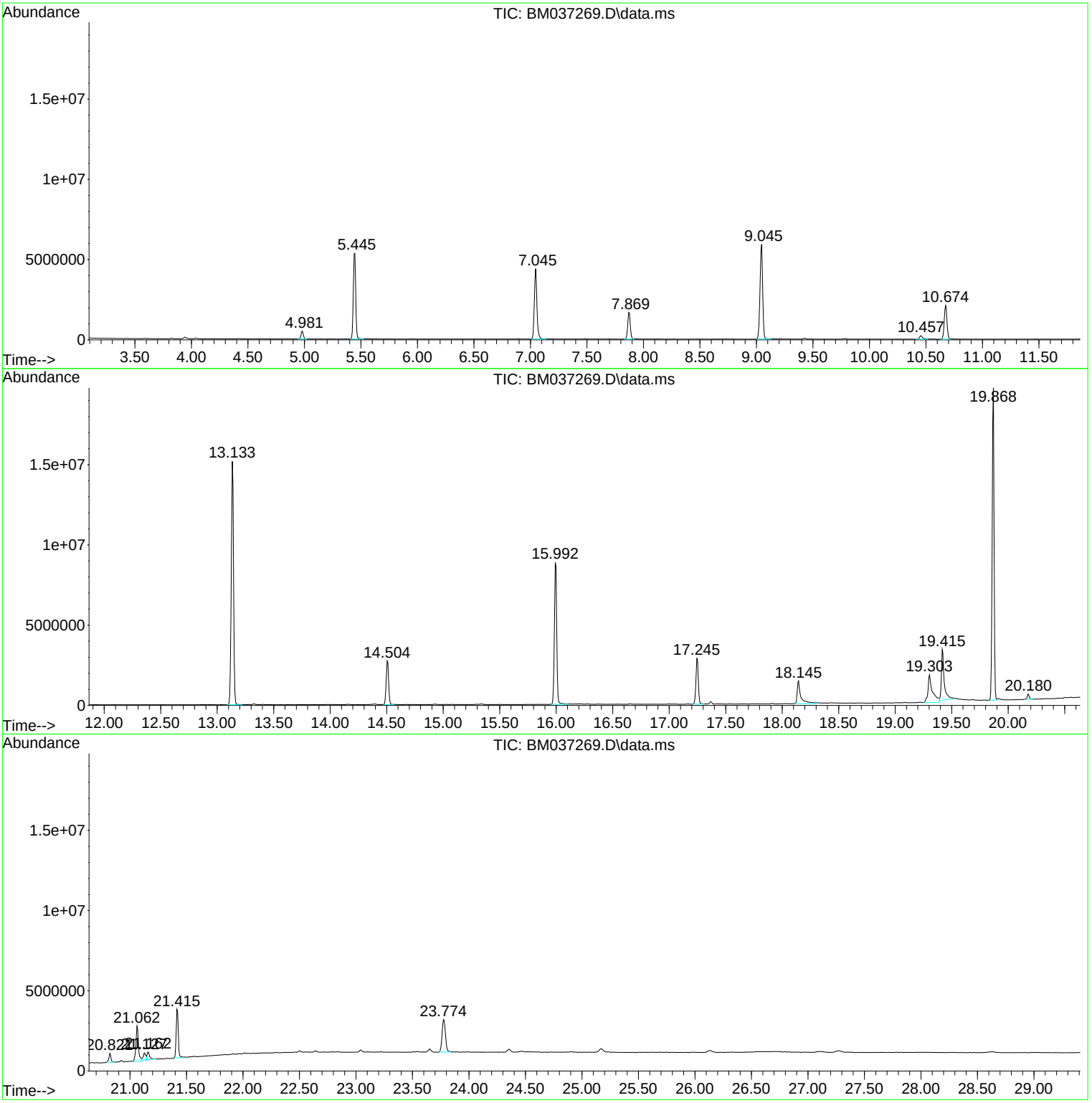
Instrument :
BNA_M
ClientSampleId :
20221099-204-SITE-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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_M\Data\BM102922\
Data File : BM037269.D
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Sample : N5266-02
Misc :
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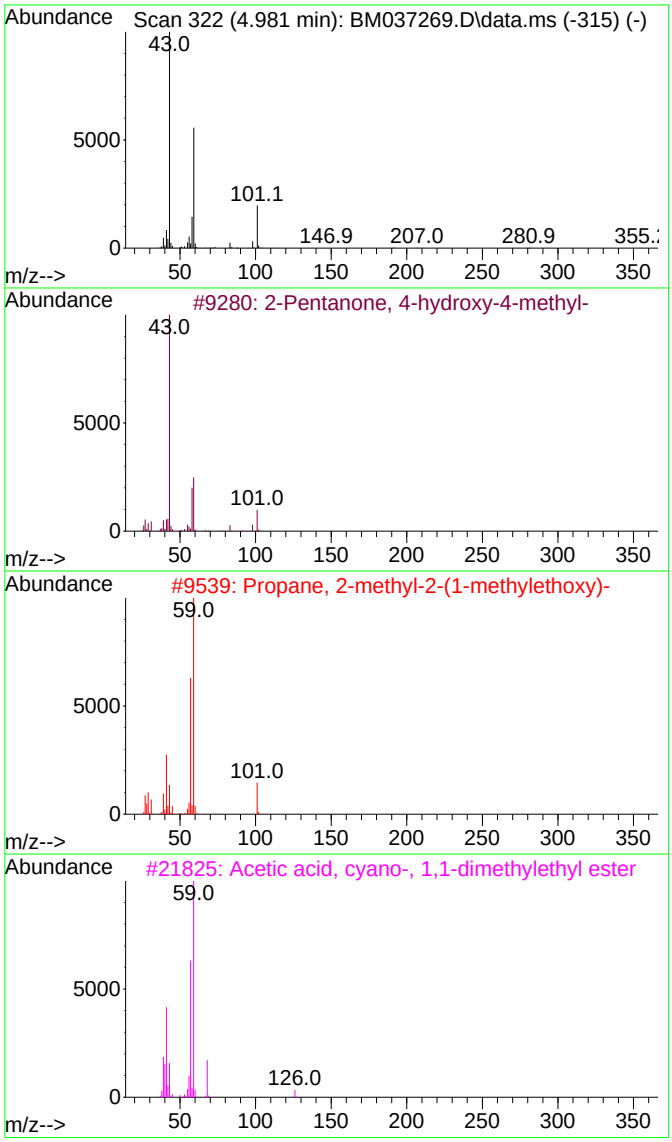
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

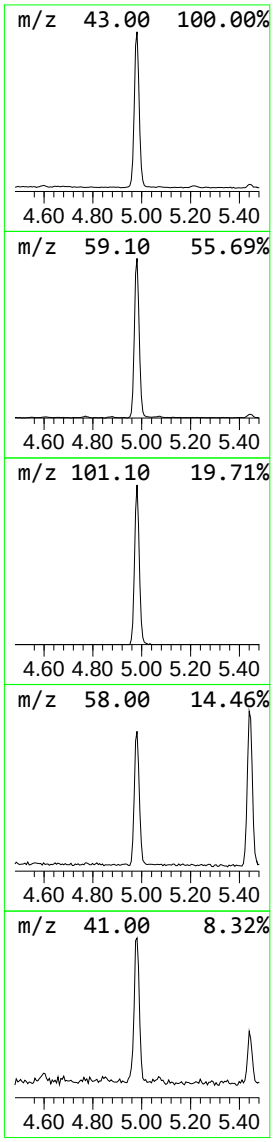
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	5.34 ng	692810	1,4-Dichlorobenzene-d4	7.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BM037269.D
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20221099-204-SITE-WATER

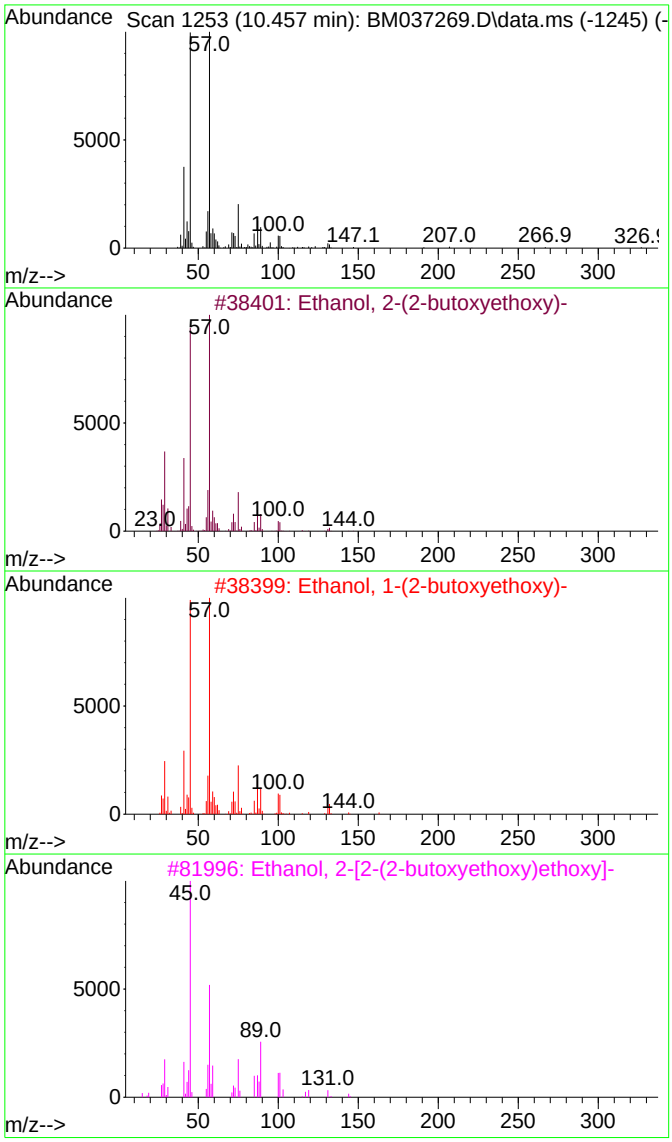
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

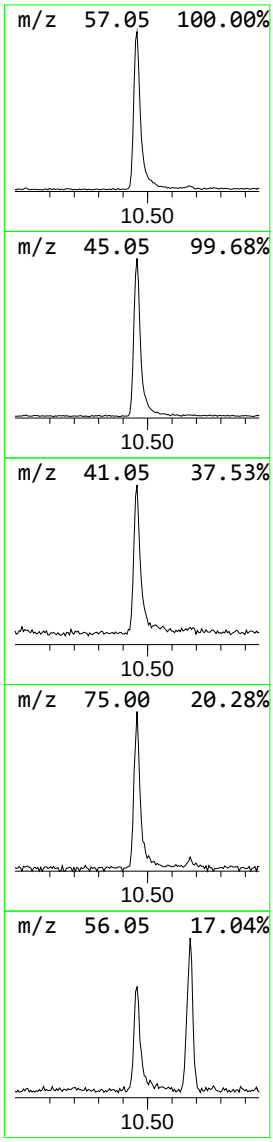
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.457	2.44 ng	420734	Naphthalene-d8	10.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	59
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53





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Operator : CG/JU
Sample : N5266-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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BNA_M
ClientSampleId :
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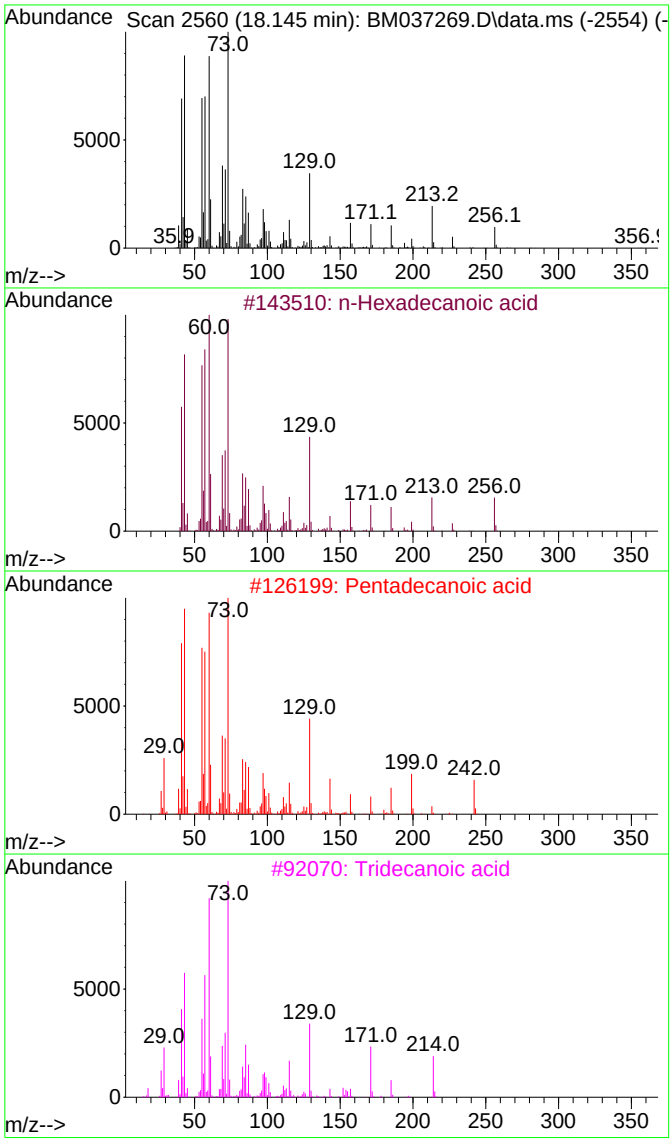
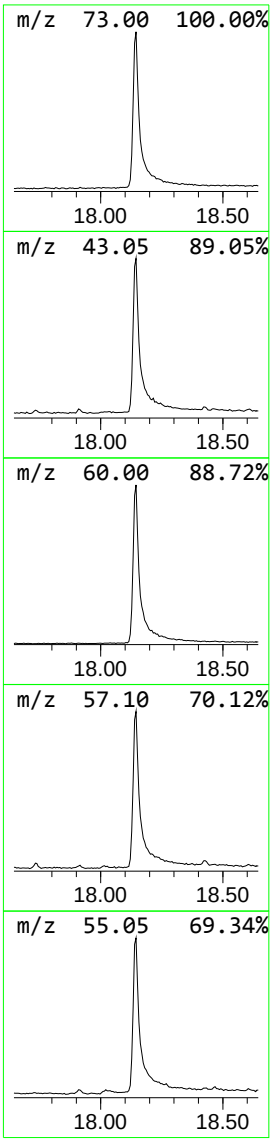
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	15.37 ng	3154870	Phenanthrene-d10	17.245

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	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Nonanoic acid	158	C9H18O2	000112-05-0	53





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Operator : CG/JU
Sample : N5266-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221099-204-SITE-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

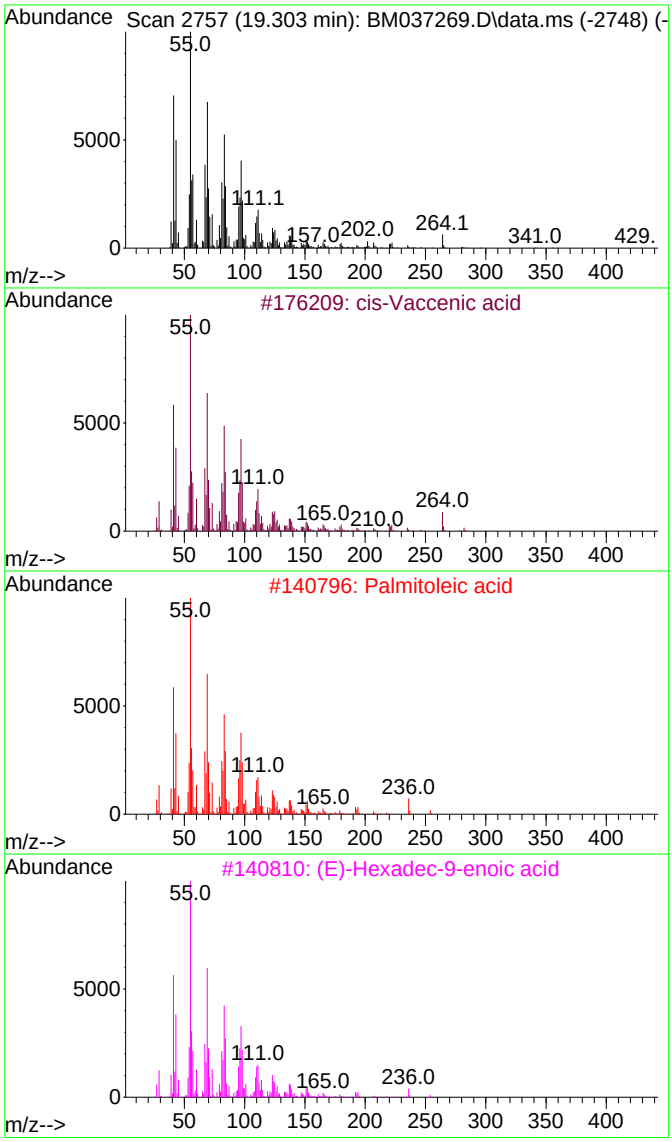
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

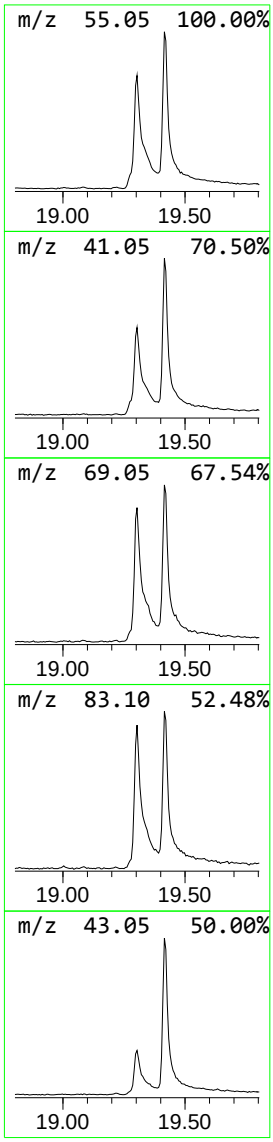
****

Peak Number 4 cis-Vaccenic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.303	23.67 ng	4858690	Phenanthrene-d10	17.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	87
2	Palmitoleic acid	254	C16H30O2	000373-49-9	87
3	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	87
4	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	87
5	4-Chloro-3-n-hexyltetrahydropyran	204	C11H21ClO	066555-66-6	76





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Sample : N5266-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
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20221099-204-SITE-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

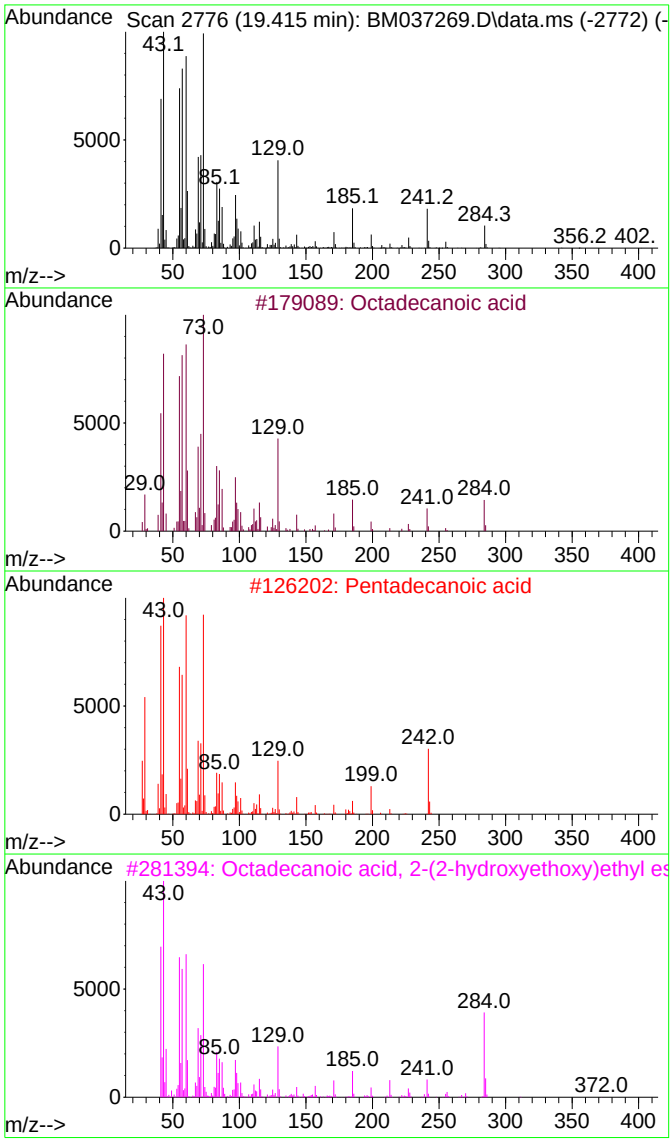
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

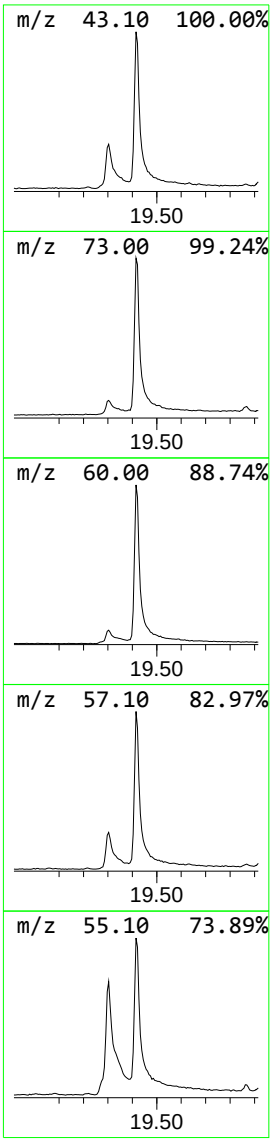
****

Peak Number 5 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.415	27.50 ng	5395820	Chrysene-d12	21.415

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	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





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Instrument :
BNA_M
ClientSampleId :
20221099-204-SITE-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

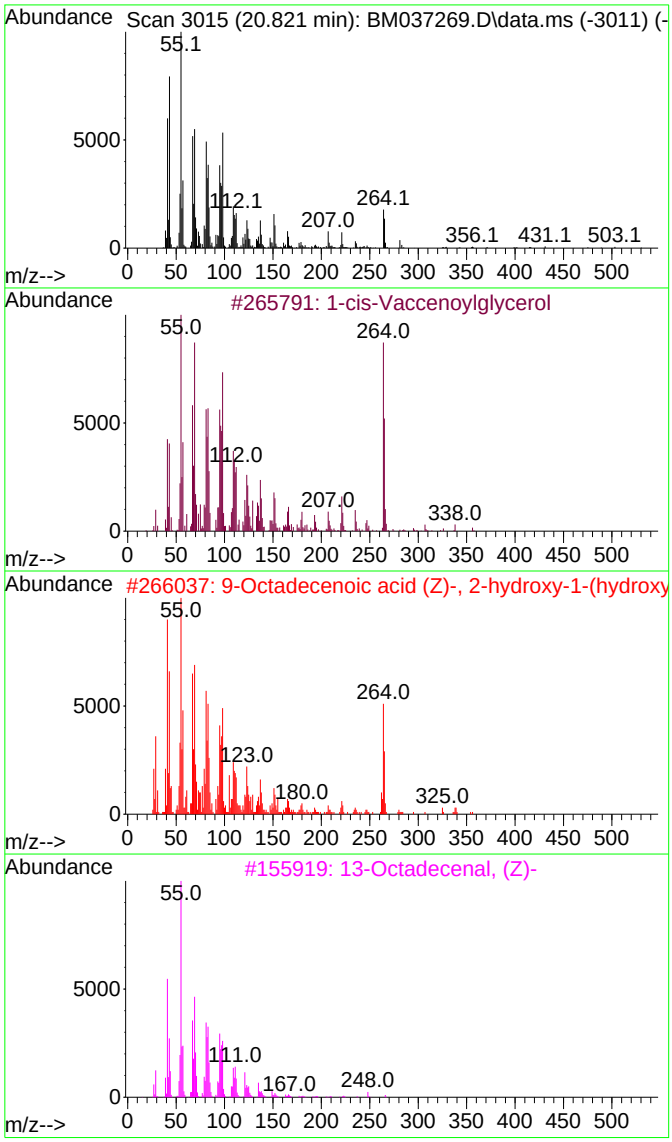
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

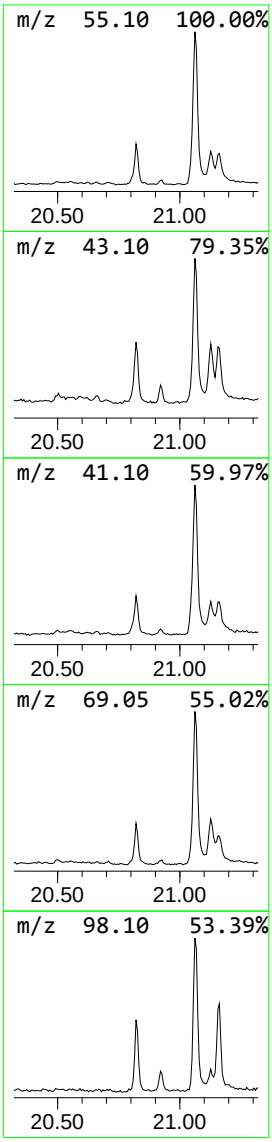
****

Peak Number 6 1-cis-Vaccenoylglycerol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.821	3.36 ng	658896	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-cis-Vaccenoylglycerol	356	C21H40O4	020379-67-3	99
2	9-Octadecenoic acid (Z)-, 2-hydr...	356	C21H40O4	003443-84-3	90
3	13-Octadecenal, (Z)-	266	C18H34O	058594-45-9	90
4	9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	78
5	9-Octadecen-1-ol, (Z)-	268	C18H36O	000143-28-2	53





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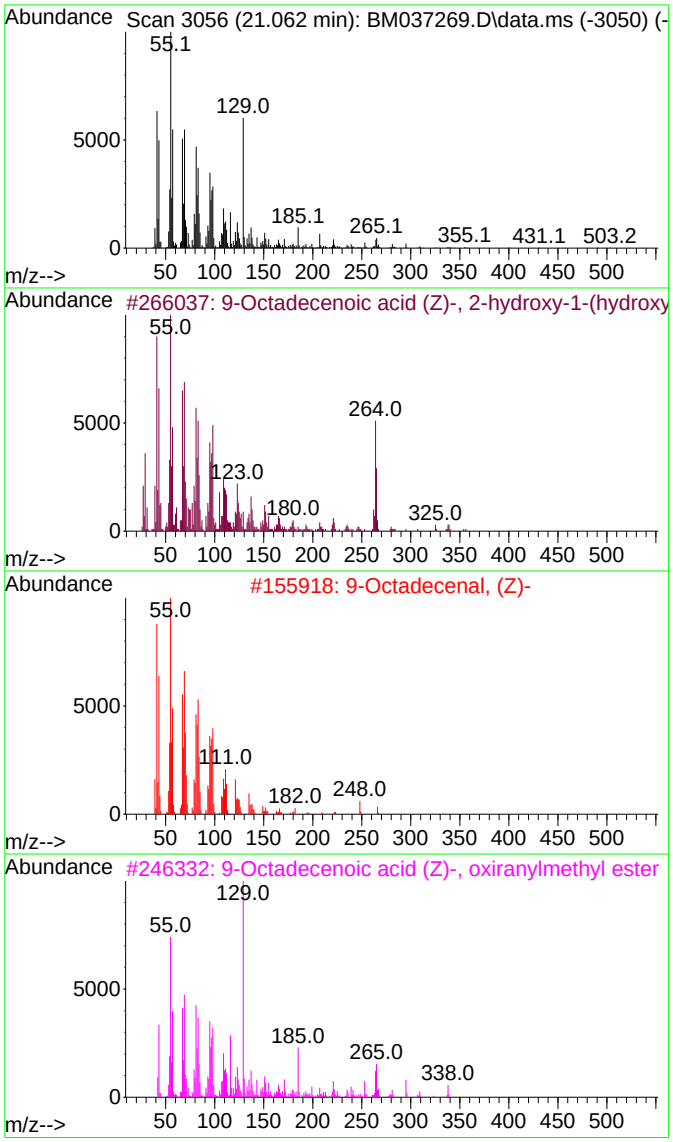
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

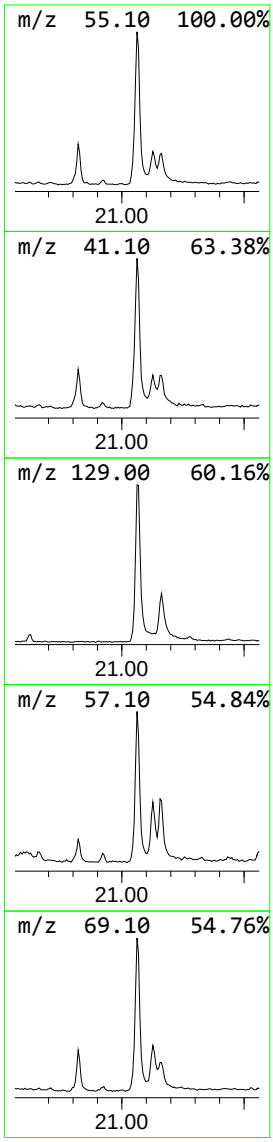
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 9-Octadecenoic acid (Z)-, 2... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.062	17.05 ng	3346550	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, 2-hydr...	356	C21H40O4	003443-84-3	98
2	9-Octadecenal, (Z)-	266	C18H34O	002423-10-1	95
3	9-Octadecenoic acid (Z)-, oxiran...	338	C21H38O3	005431-33-4	91
4	9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	90
5	Glycidyl (Z)-9-Heptadecenoate	324	C20H36O3	1000465-63-2	83





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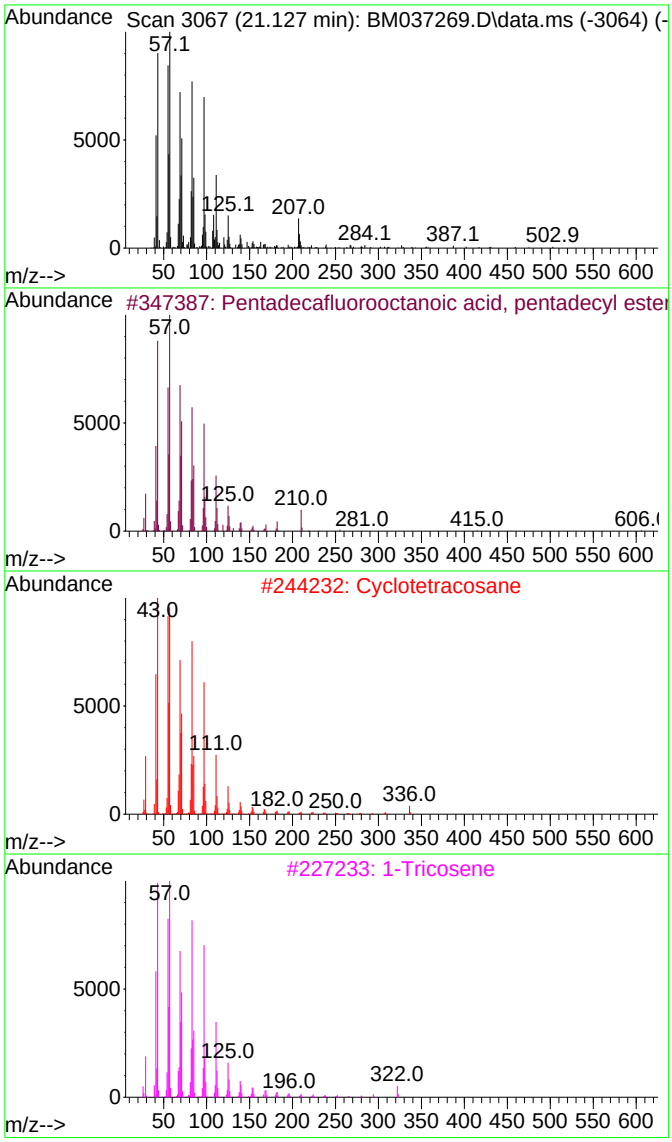
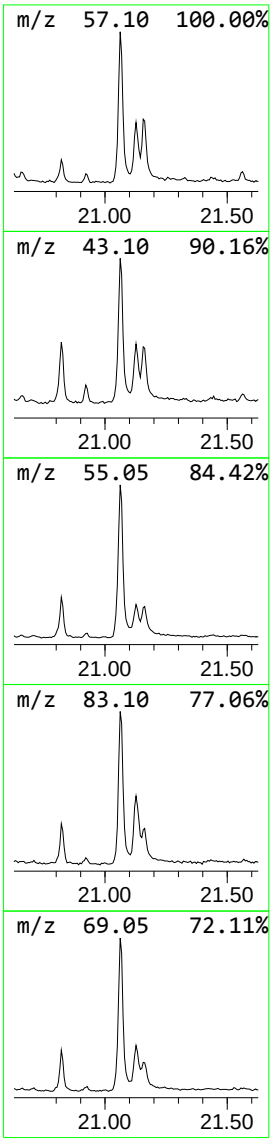
****
Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	3.39 ng	665619	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	93
2	Cyclotetracosane	336	C24H48	000297-03-0	90
3	1-Tricosene	322	C23H46	018835-32-0	90
4	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	90
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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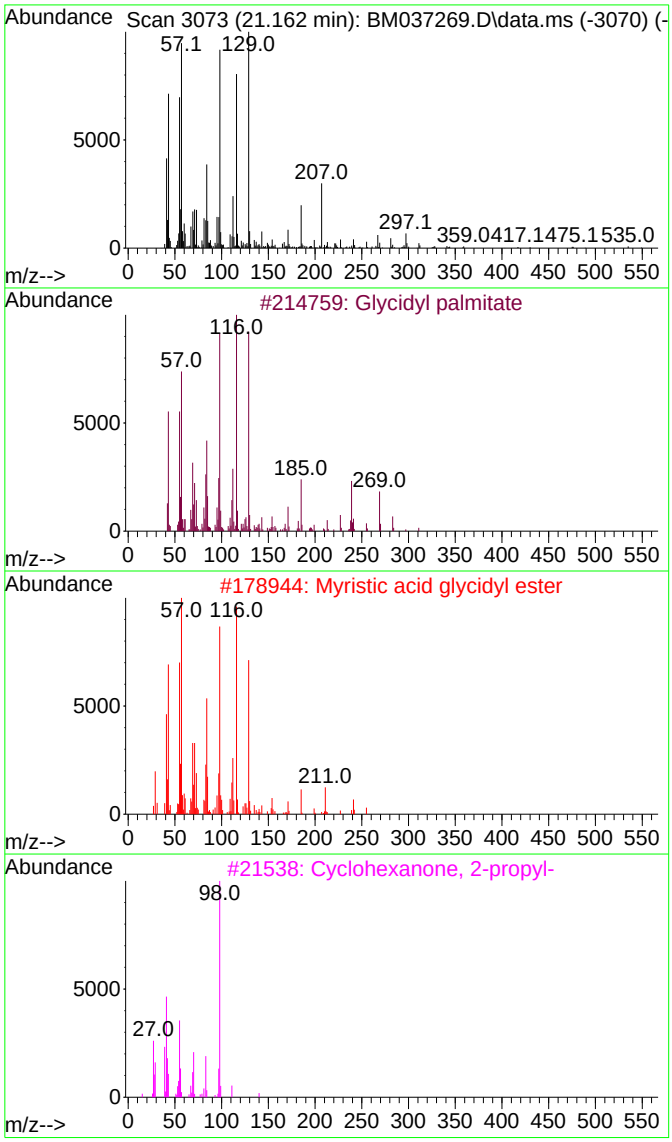
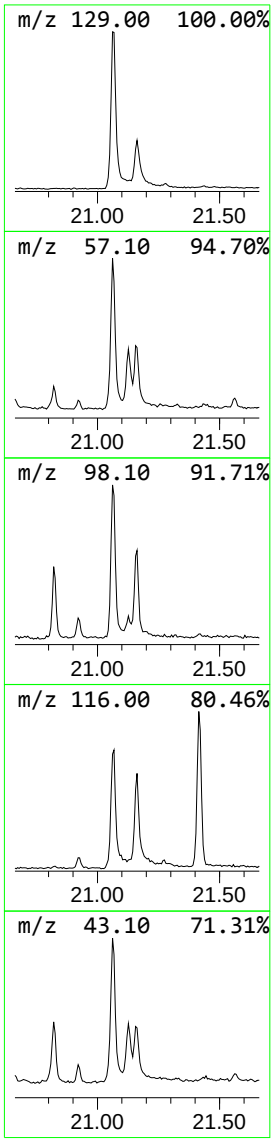
****

Peak Number 9 unknown21.162 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.162	3.92 ng	769341	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glycidyl palmitate	312	C19H36O3	007501-44-2	47
2	Myristic acid glycidyl ester	284	C17H32O3	007460-80-2	47
3	Cyclohexanone, 2-propyl-	140	C9H16O	000094-65-5	25
4	Hexanoic acid, 4-oxo-6-(1-piperi...	213	C11H19NO3	339313-13-2	18
5	3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102922\
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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-...	4.981	5.3	ng	692810	1	7.875	2594400	20.0
Ethanol, 2-(2-b...	10.457	2.4	ng	420734	2	10.675	3443430	20.0
n-Hexadecanoic ...	18.145	15.4	ng	3154870	4	17.245	4104700	20.0
cis-Vaccenic acid	19.303	23.7	ng	4858690	4	17.245	4104700	20.0
Octadecanoic acid	19.415	27.5	ng	5395820	5	21.415	3924940	20.0
1-cis-Vaccenoyl...	20.821	3.4	ng	658896	5	21.415	3924940	20.0
9-Octadecenoic ...	21.062	17.1	ng	3346550	5	21.415	3924940	20.0
Pentadecafluoro...	21.127	3.4	ng	665619	5	21.415	3924940	20.0
unknown21.162	21.162	3.9	ng	769341	5	21.415	3924940	20.0