LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132481.D
Acq On : 20 Feb 2023 15:51
Operator : CG\JU
Sample : 01593-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SW-1

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-BF021623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132481.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.231	402	407	408	rBV	114069	108341	1.82%	0.265%
2	5.260	408	412	424	rVB	1440770	1687556	28.32%	4.120%
3	5.654	474	479	482	rBV	3923086	4055763	68.06%	9.903%
4	6.643	642	647	650	rBV	3431910	3152212	52.90%	7.696%
5	7.025	708	712	715	rBV	1642273	1283437	21.54%	3.134%
6	7.590	803	808	811	rBV	4002916	3641846	61.11%	8.892%
7	8.313	927	931	934	rBV	1826209	1618128	27.15%	3.951%
8	9.389	1110	1114	1117	rVB	6800463	5959228	100.00%	14.550%
9	10.072	1227	1230	1234	rVB	1926536	1642617	27.56%	4.011%
10	10.789	1348	1352	1355	rVB	1713854	1370769	23.00%	3.347%
11	10.866	1361	1365	1369	rBV	3283802	3304346	55.45%	8.068%
12	11.213	1421	1424	1429	rBV	124418	129946	2.18%	0.317%
13	11.572	1481	1485	1488	rBV	1572080	1460121	24.50%	3.565%
14	12.001	1556	1558	1564	rBV	138308	173341	2.91%	0.423%
15	12.083	1568	1572	1588	rVV	1322984	1419144	23.81%	3.465%
16	12.477	1636	1639	1641	rBV2	77467	67007	1.12%	0.164%
17	12.501	1641	1643	1646	rVB	192529	143475	2.41%	0.350%
18	12.789	1687	1692	1700	rBV4	103806	181418	3.04%	0.443%
19	12.866	1702	1705	1716	rVV	286093	386242	6.48%	0.943%
20	13.160	1751	1755	1758	rBV	4986264	4664222	78.27%	11.388%
21	14.060	1904	1908	1924	rBV2	234276	773269	12.98%	1.888%
22	14.224	1933	1936	1940	rBV	1133187	1031356	17.31%	2.518%
23	14.319	1948	1952	1956	rVB	371325	366202	6.15%	0.894%
24	15.095	2080	2084	2088	rVB	1547031	1568856	26.33%	3.831%
25	15.789	2198	2202	2207	rVB	602929	768105	12.89%	1.875%

Sum of corrected areas: 40956947

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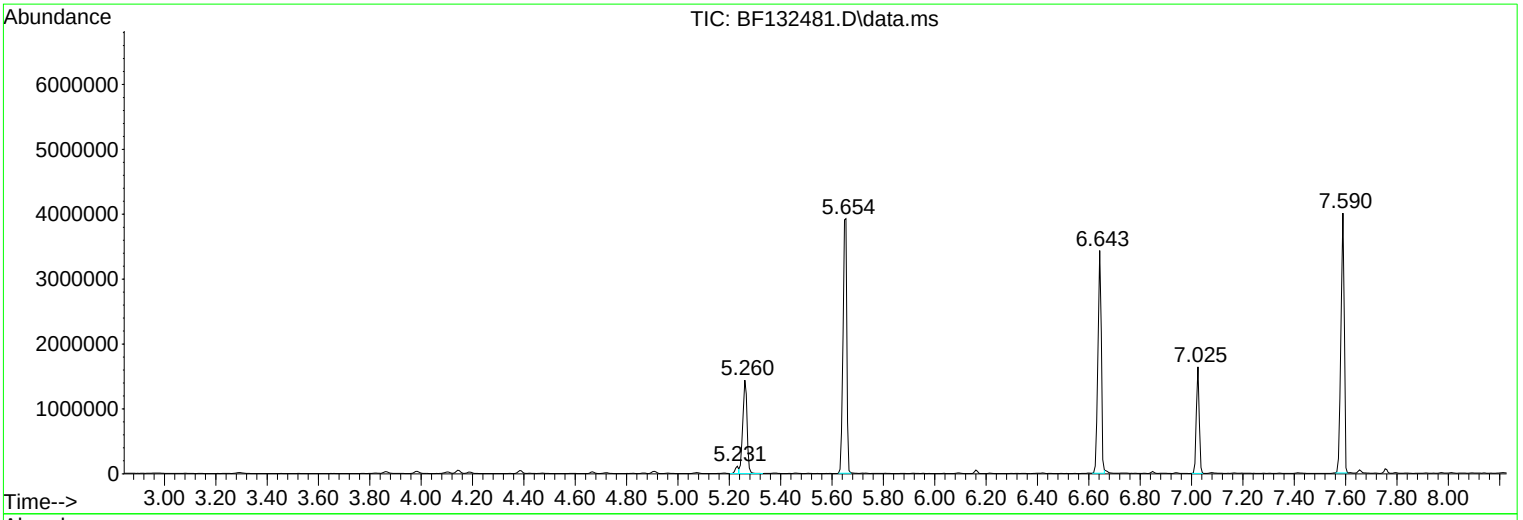
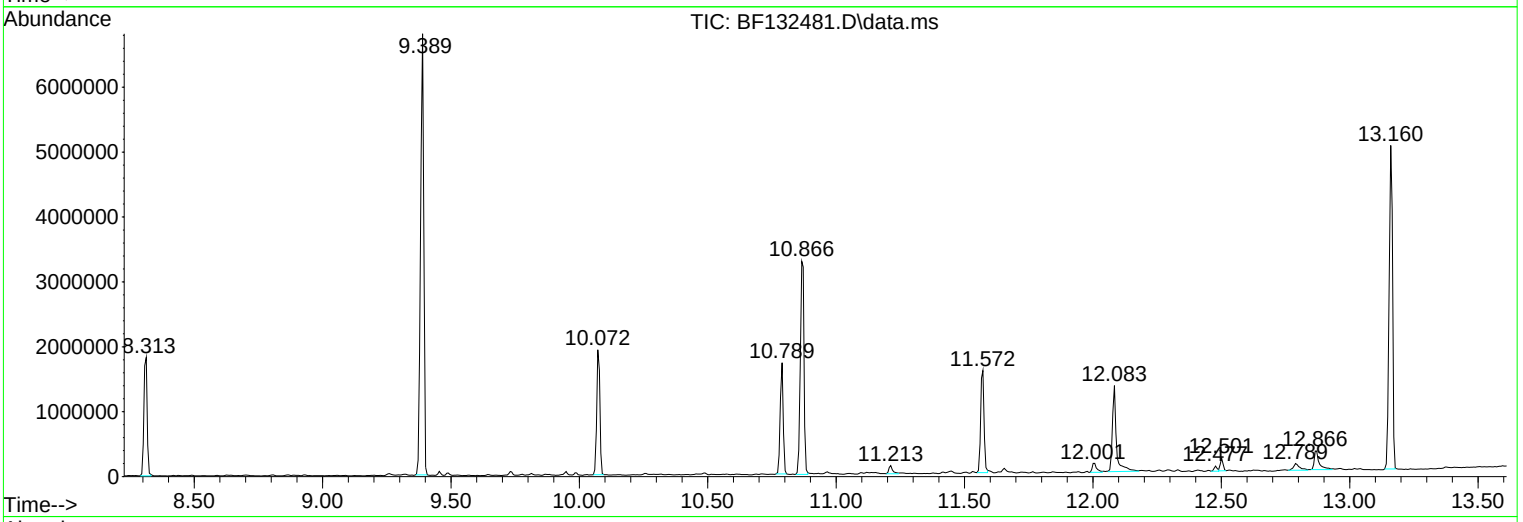
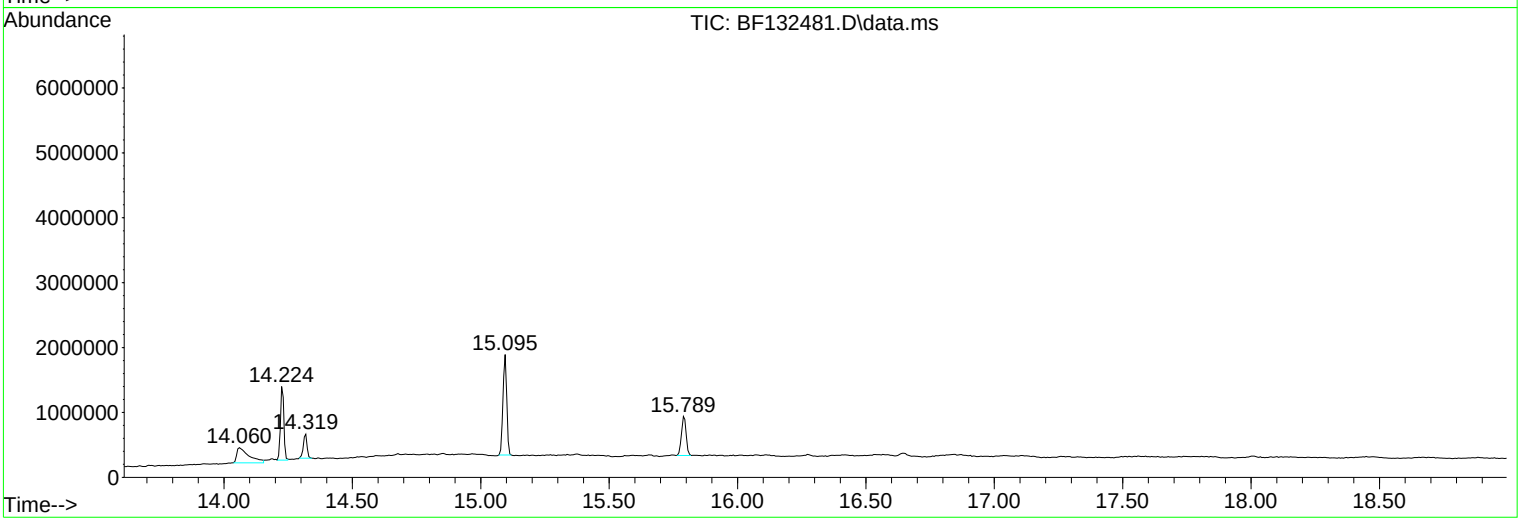
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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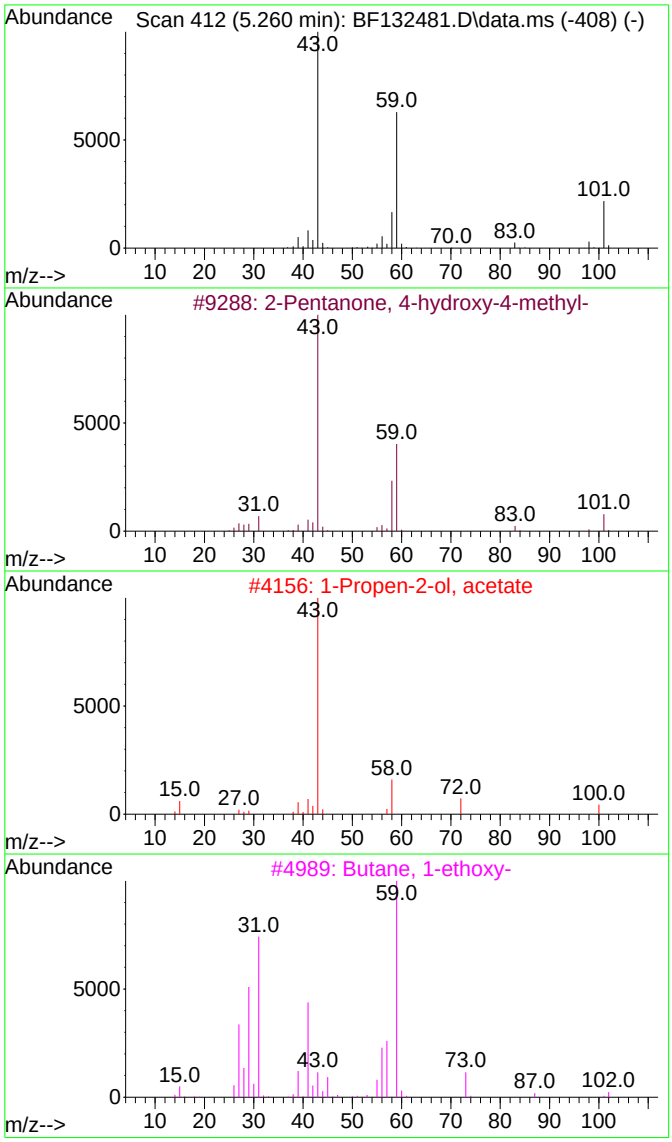
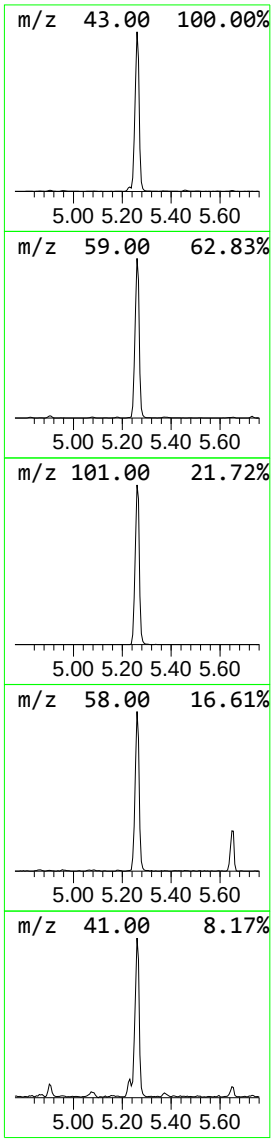
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.260	26.30 ng	1687560	1,4-Dichlorobenzene-d4	7.025

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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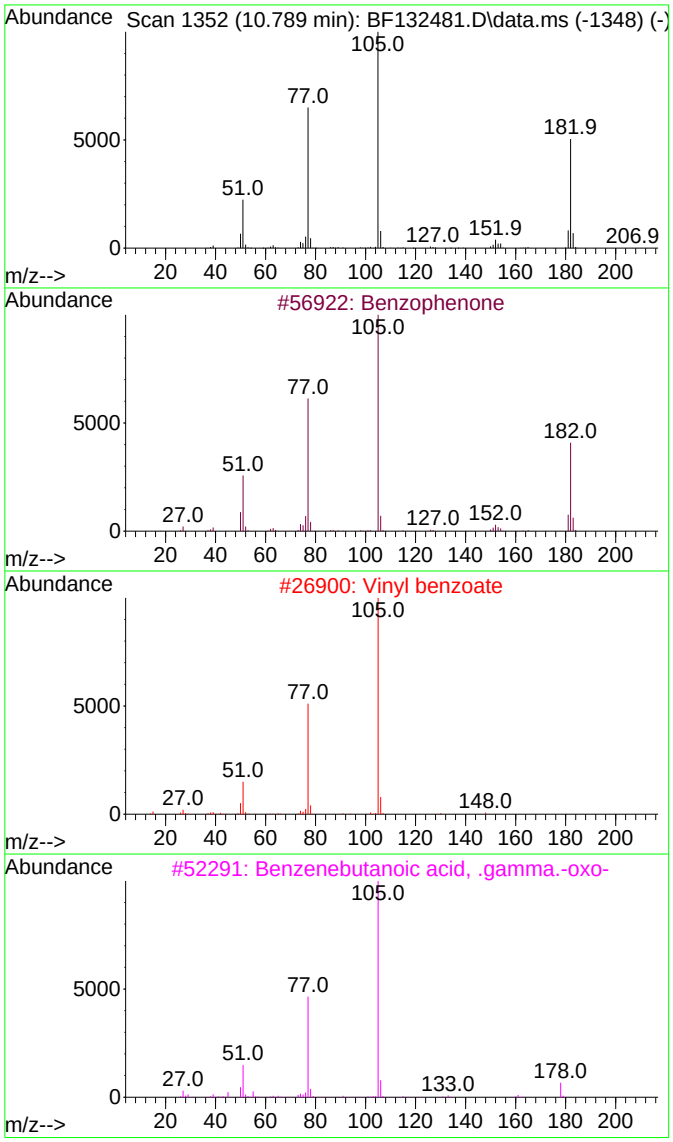
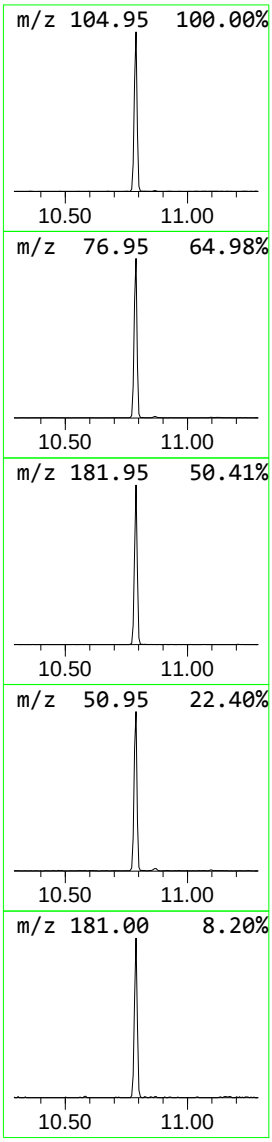
****

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.789	16.69 ng	1370770	Acenaphthene-d10	10.072

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Vinyl benzoate	148	C9H8O2	000769-78-8	47
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47





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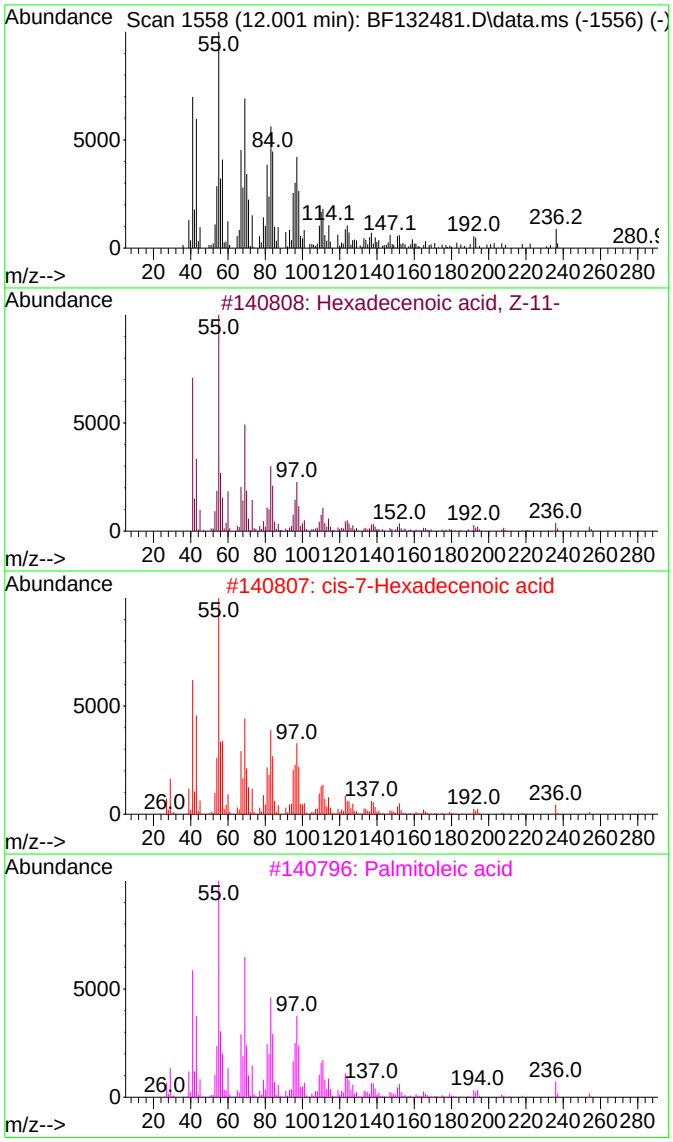
TIC Integration Parameters: LSCINT.P

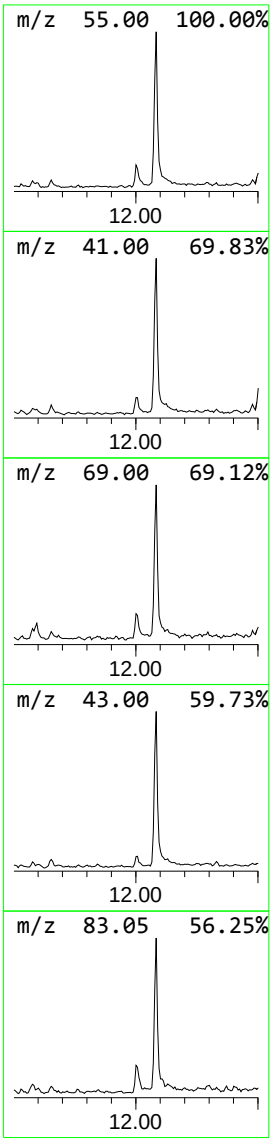
****

Peak Number 3 Hexadecenoic acid, Z-11- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.001	2.37 ng	173341	Phenanthrene-d10	11.572

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	87
2	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	70
3	Palmitoleic acid	254	C16H30O2	000373-49-9	68
4	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	64
5	trans-2-methyl-4-n-pentylthiane,...	218	C11H22O2S	1000215-75-3	49





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

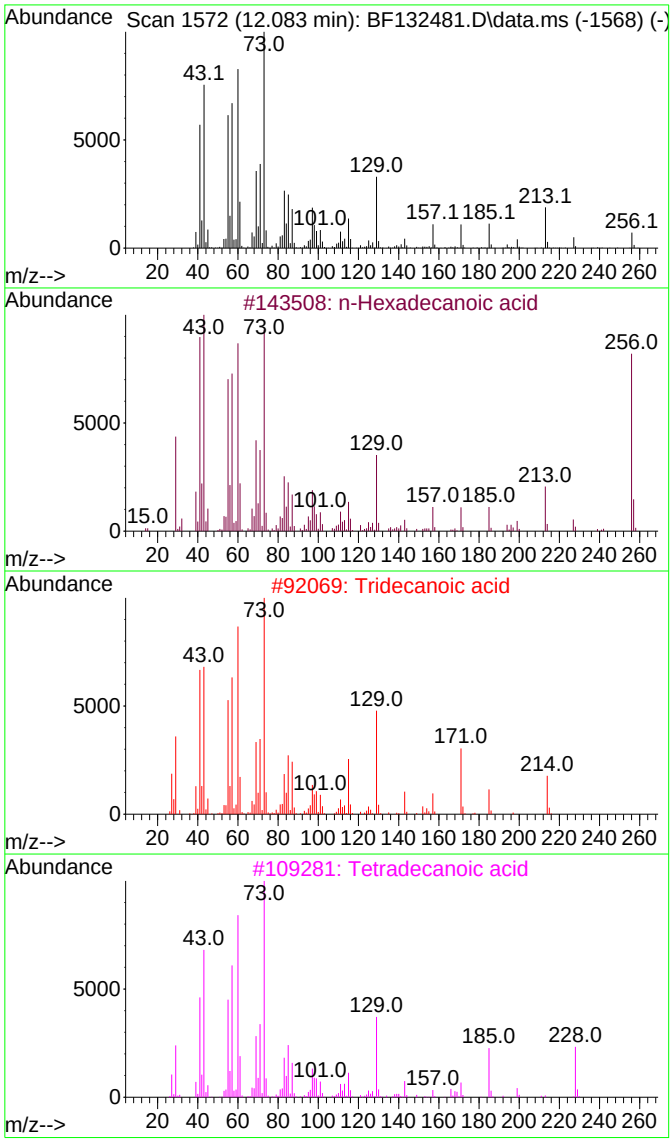
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

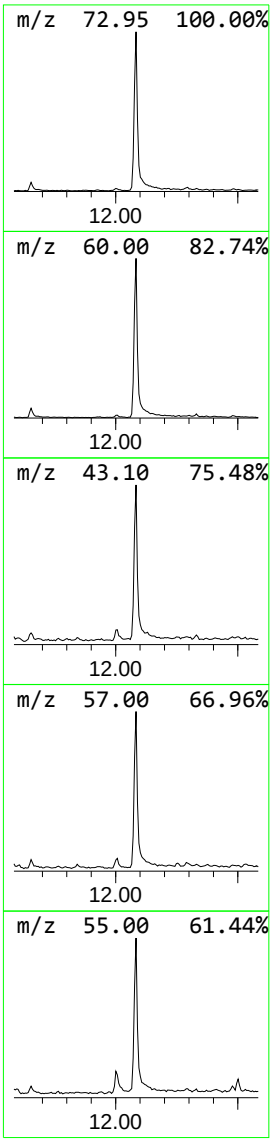
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.083	19.44 ng	1419140	Phenanthrene-d10	11.572

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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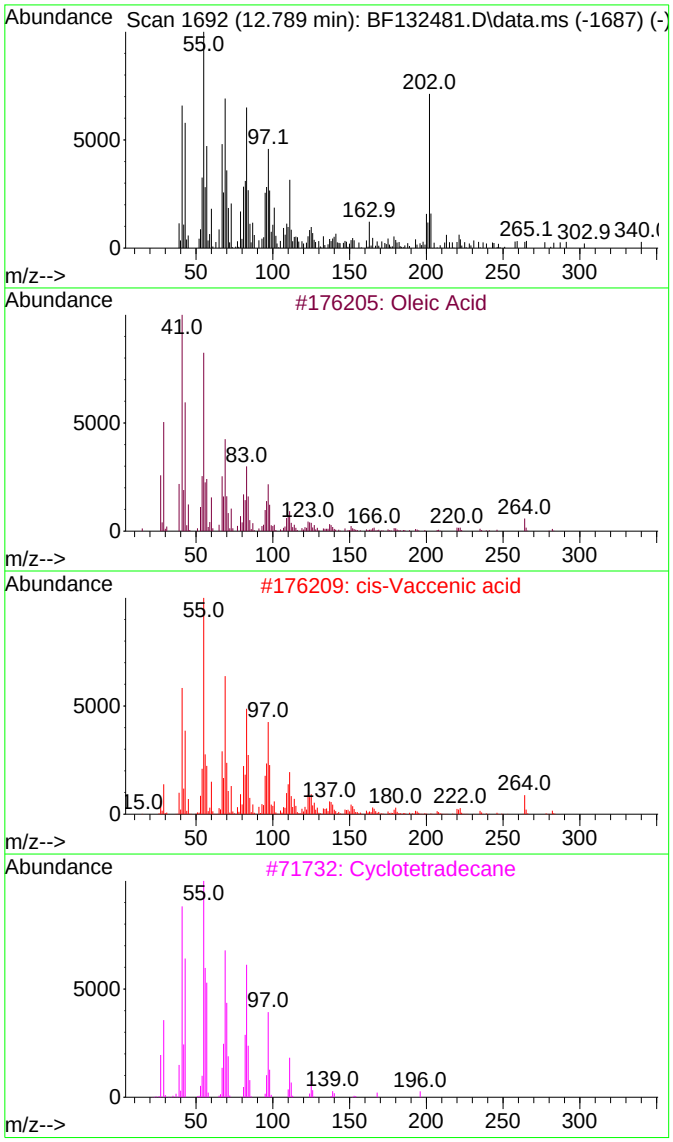
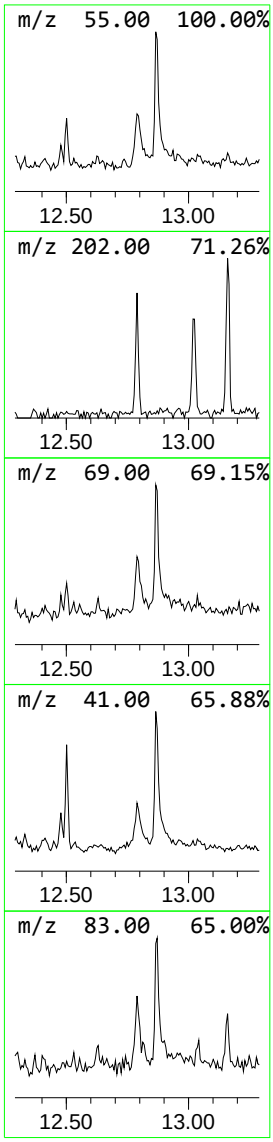
Peak Number 5 Oleic Acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.789	2.48 ng	181418	Phenanthrene-d10	11.572

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	83
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	58
3	Cyclotetradecane	196	C14H28	000295-17-0	53
4	13-Tetradecenal	210	C14H26O	085896-31-7	50
5	1-Hexadecanol	242	C16H34O	036653-82-4	46





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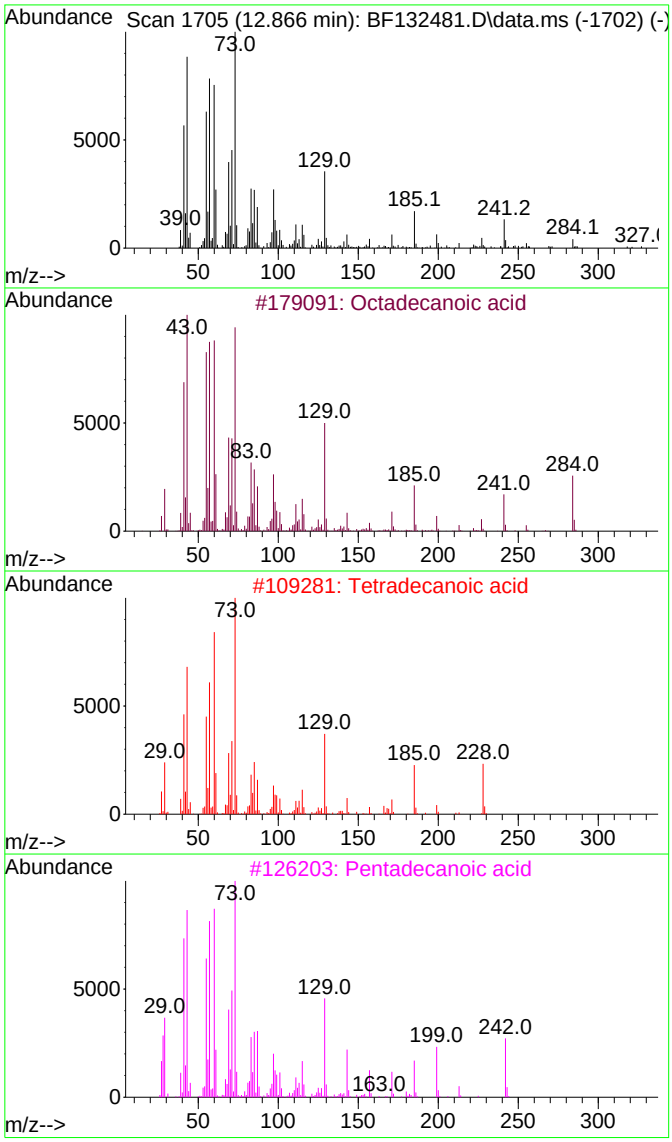
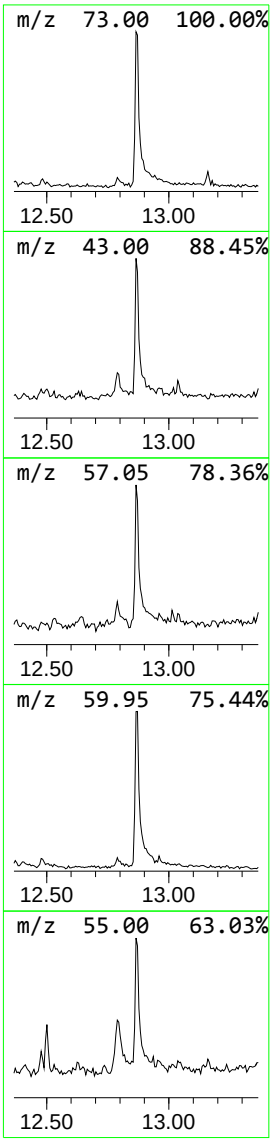
****

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.866	5.29 ng	386242	Phenanthrene-d10	11.572

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46





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TIC Library : C:\Database\NIST20.L
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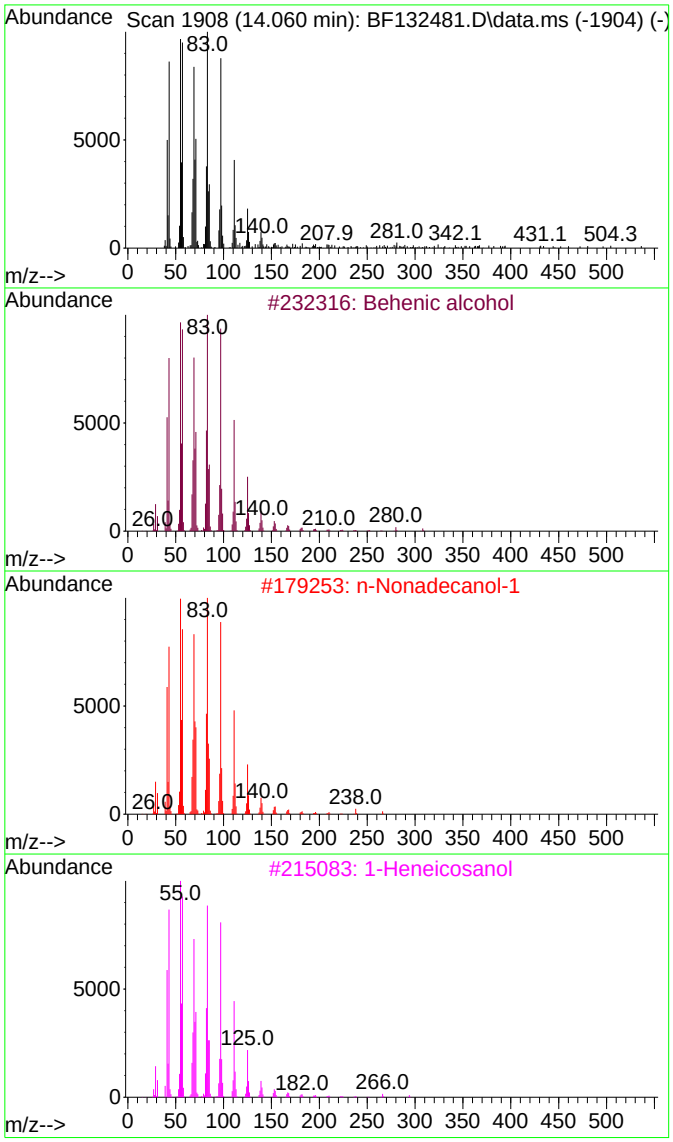
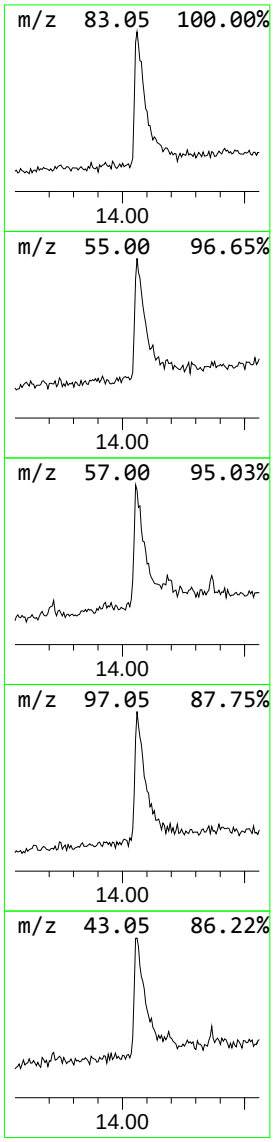
Peak Number 7 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.060	15.00 ng	773269	Chrysene-d12	14.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





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TIC Library : C:\Database\NIST20.L
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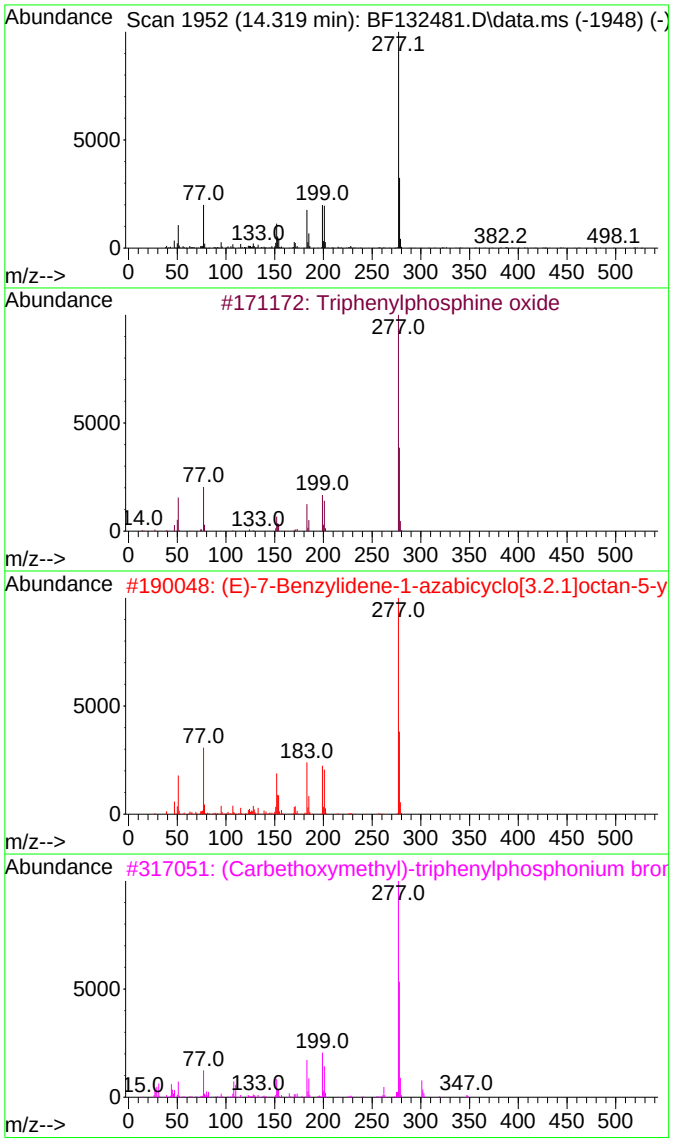
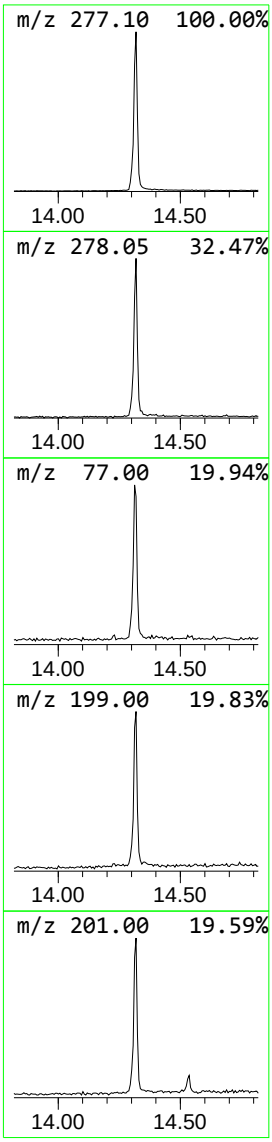
Peak Number 8 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.319	7.10 ng	366202	Chrysene-d12	14.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	52
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50
4	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	38
5	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	33





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

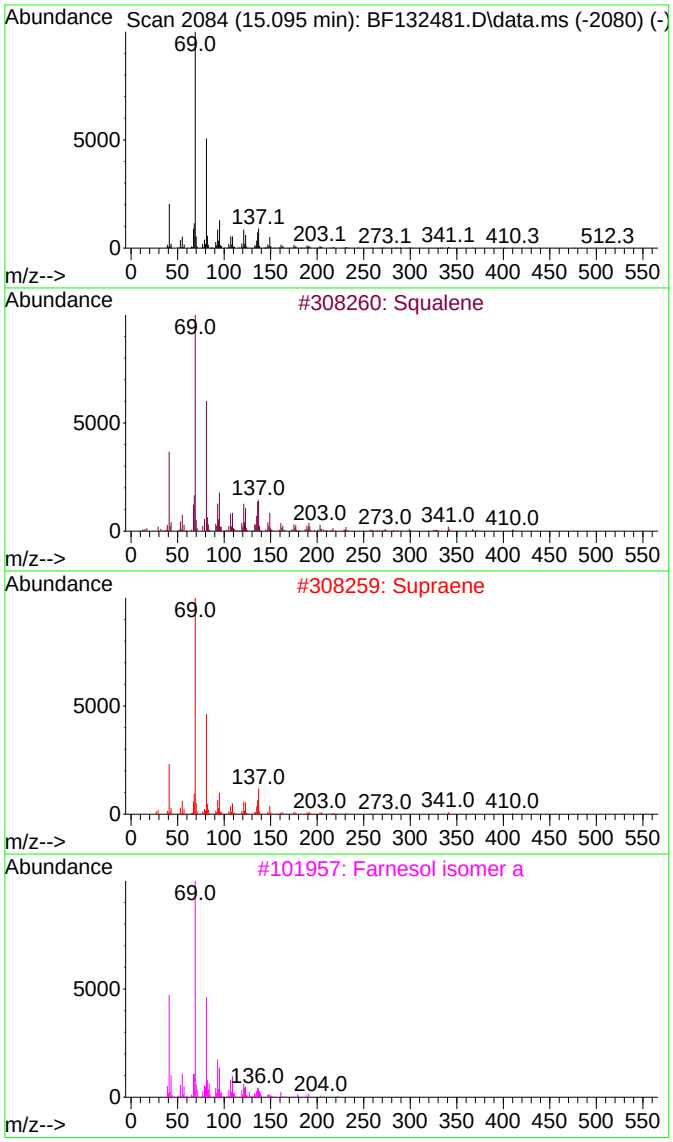
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

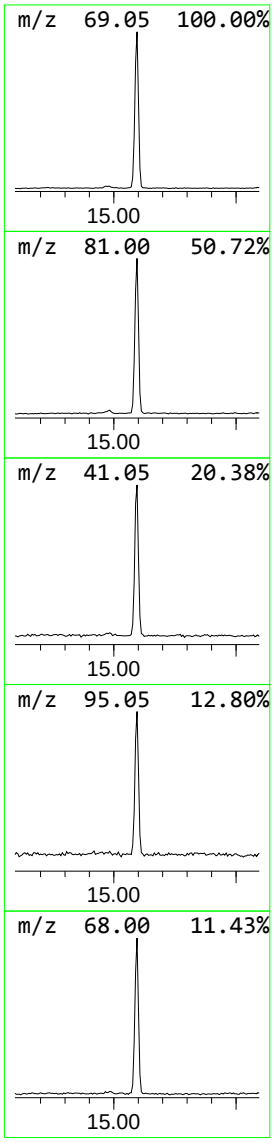
****

Peak Number 9 Squalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.095	40.85 ng	1568860	Perylene-d12	15.789

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	94
2	Supraene	410	C30H50	007683-64-9	91
3	Farnesol isomer a	222	C15H26O	1000108-92-4	64
4	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50





Tentatively Identified Compound (LSC) summary

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ClientSampleId :
SW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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-...	5.260	26.3	ng	1687560	1	7.025	1283440	20.0
Benzophenone	10.789	16.7	ng	1370770	3	10.072	1642620	20.0
Hexadecenoic ac...	12.001	2.4	ng	173341	4	11.572	1460120	20.0
n-Hexadecanoic ...	12.083	19.4	ng	1419140	4	11.572	1460120	20.0
Oleic Acid	12.789	2.5	ng	181418	4	11.572	1460120	20.0
Octadecanoic acid	12.866	5.3	ng	386242	4	11.572	1460120	20.0
Behenic alcohol	14.060	15.0	ng	773269	5	14.224	1031360	20.0
Triphenylphosph...	14.319	7.1	ng	366202	5	14.224	1031360	20.0
Squalene	15.095	40.9	ng	1568860	6	15.789	768105	20.0