LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130380.D
Acq On : 22 Sep 2022 17:32
Operator : CG\JU
Sample : N4609-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DSN002

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-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130380.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.834	463	467	475	rVB	104132	112464	3.60%	0.585%
2	5.257	535	539	551	rBV	1481504	1431928	45.81%	7.451%
3	6.292	711	715	731	rVB	850233	949333	30.37%	4.940%
4	6.657	773	777	780	rBV	723879	638088	20.42%	3.320%
5	7.222	868	873	876	rBV	1957456	1830854	58.58%	9.527%
6	7.416	902	906	910	rVB2	67237	64126	2.05%	0.334%
7	7.857	978	981	991	rBV	359919	951572	30.45%	4.952%
8	7.939	991	995	998	rVB	845514	839762	26.87%	4.370%
9	8.310	1053	1058	1061	rBV2	42174	58596	1.87%	0.305%
10	8.822	1141	1145	1148	rBV	47561	44831	1.43%	0.233%
11	9.016	1172	1178	1181	rBV	3817039	3125515	100.00%	16.264%
12	9.145	1195	1200	1215	rVB	260892	394514	12.62%	2.053%
13	9.686	1285	1292	1295	rBV	973002	764468	24.46%	3.978%
14	9.845	1316	1319	1324	rBV	73746	81555	2.61%	0.424%
15	10.192	1374	1378	1385	rVB6	23820	38071	1.22%	0.198%
16	10.474	1422	1426	1429	rBV	1934364	1587056	50.78%	8.258%
17	10.592	1444	1446	1455	rVB	31911	48882	1.56%	0.254%
18	10.933	1501	1504	1509	rVB	177339	144340	4.62%	0.751%
19	11.045	1519	1523	1525	rBV2	42019	37419	1.20%	0.195%
20	11.168	1540	1544	1547	rBV	736560	619050	19.81%	3.221%
21	11.568	1608	1612	1615	rBV	210153	186776	5.98%	0.972%
22	11.710	1632	1636	1648	rBV2	508804	531062	16.99%	2.763%
23	12.274	1726	1732	1739	rVB	356719	349076	11.17%	1.816%
24	12.362	1744	1747	1750	rVB	90453	71108	2.28%	0.370%
25	12.421	1751	1757	1766	rBV	30099	81861	2.62%	0.426%
26	12.492	1766	1769	1774	rBV	117343	133020	4.26%	0.692%
27	12.680	1798	1801	1804	rVB	73740	64867	2.08%	0.338%
28	12.757	1809	1814	1817	rBV	2913918	2491637	79.72%	12.966%
29	13.798	1987	1991	1996	rBV	723885	620420	19.85%	3.228%
30	13.904	2004	2009	2012	rBV	212451	240568	7.70%	1.252%
31	14.645	2131	2135	2139	rBV2	145124	137843	4.41%	0.717%
32	15.192	2223	2228	2232	rBV	494303	546707	17.49%	2.845%

Sum of corrected areas: 19217369

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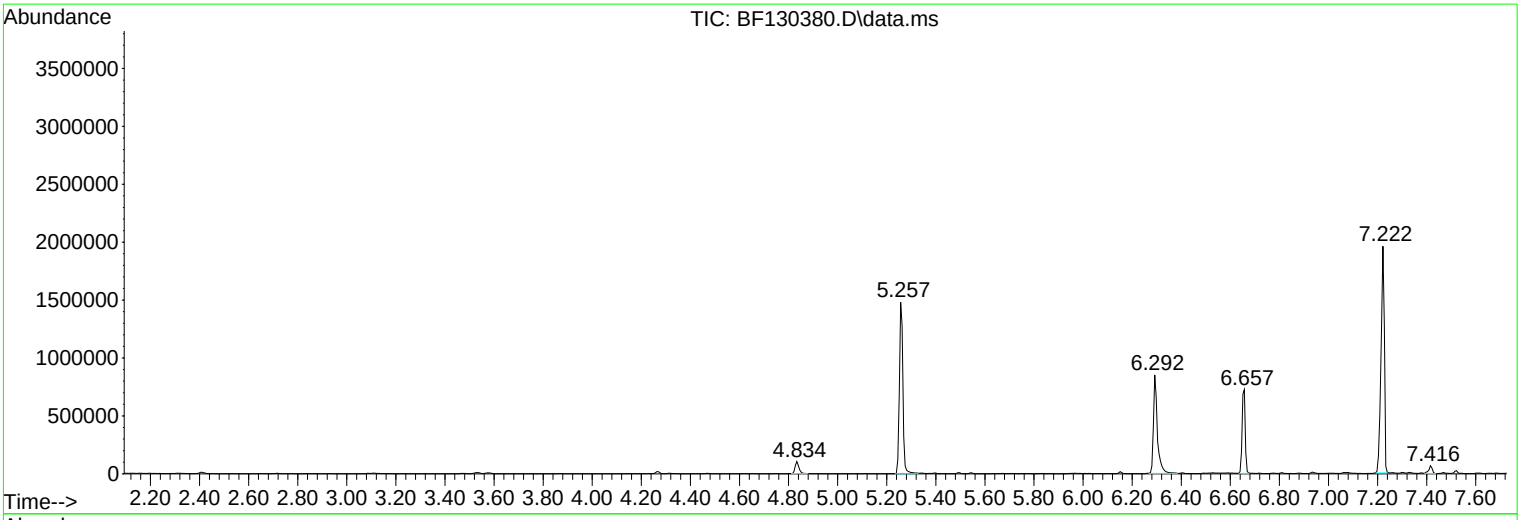
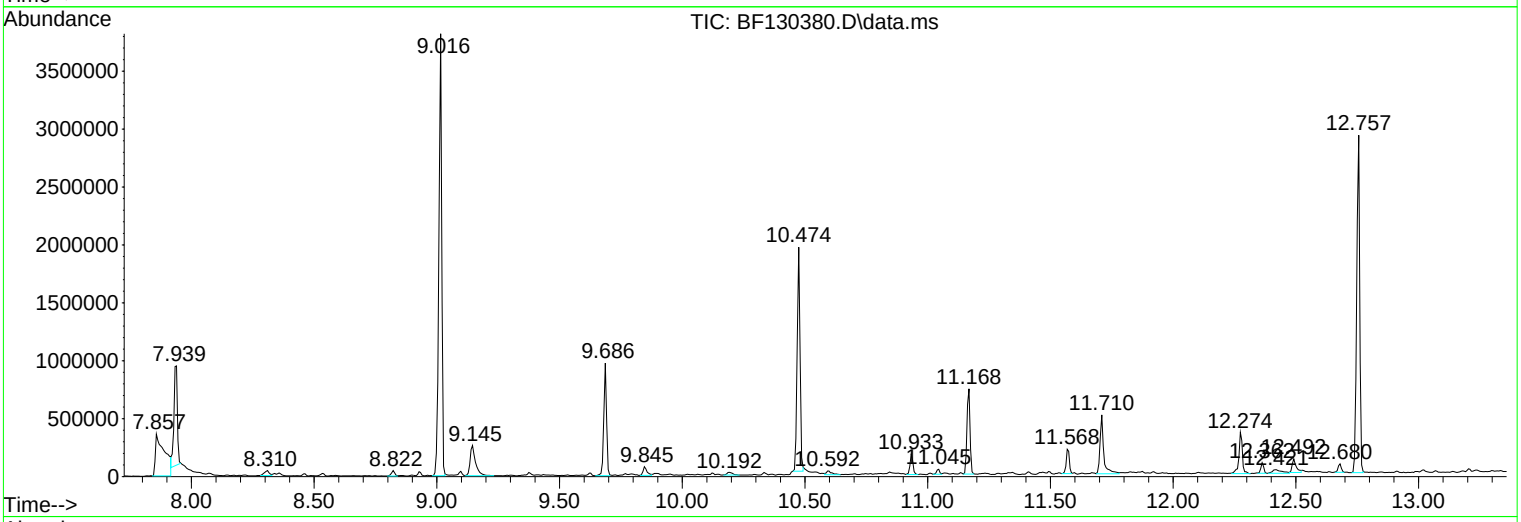
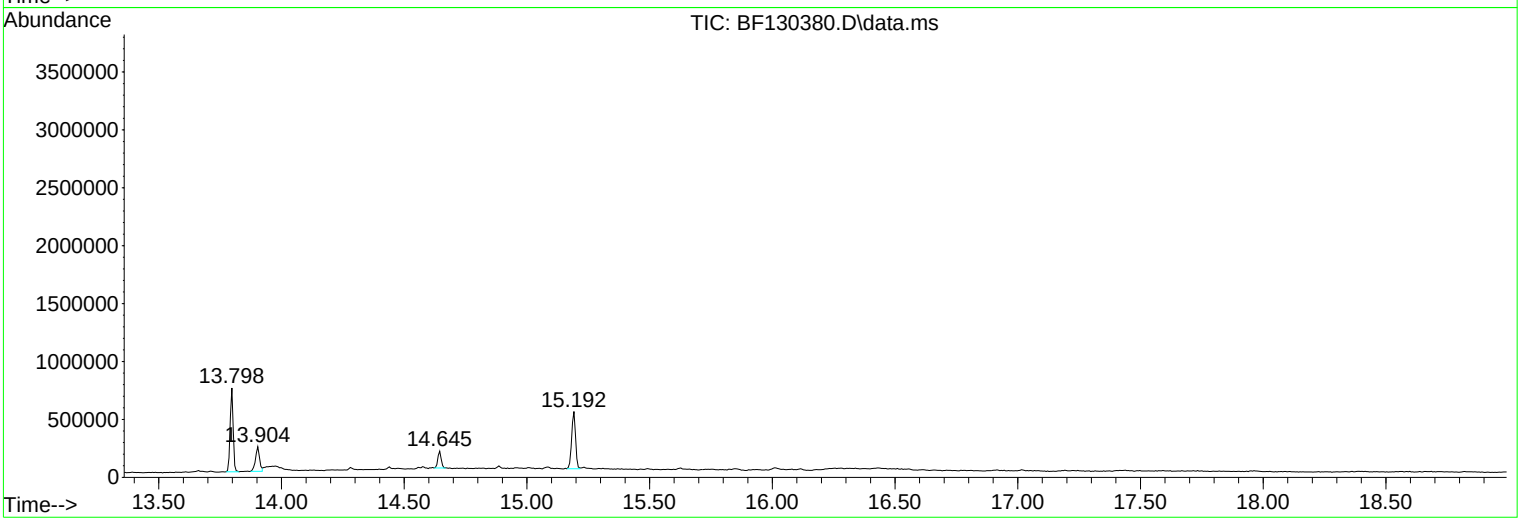
ClientSampleId :
DSN002

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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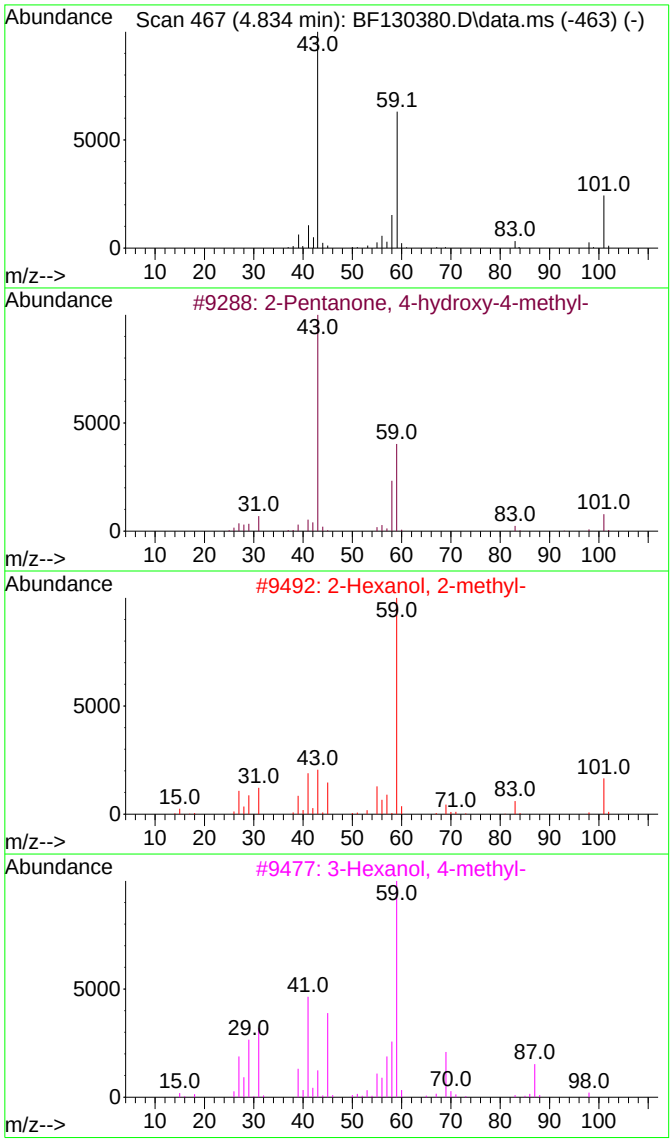
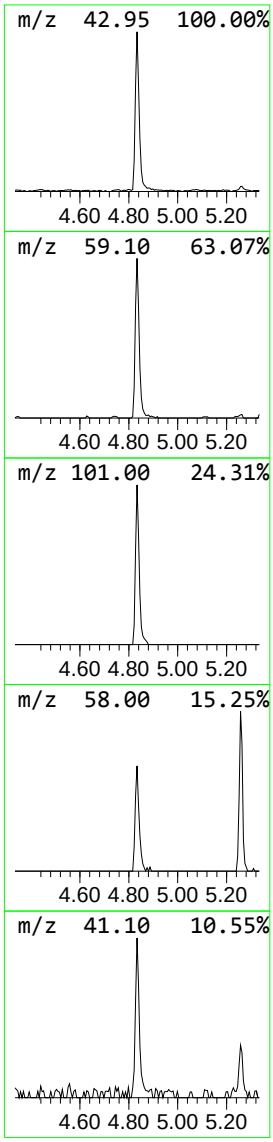
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.834	3.53 ng	112464	1,4-Dichlorobenzene-d4	6.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25





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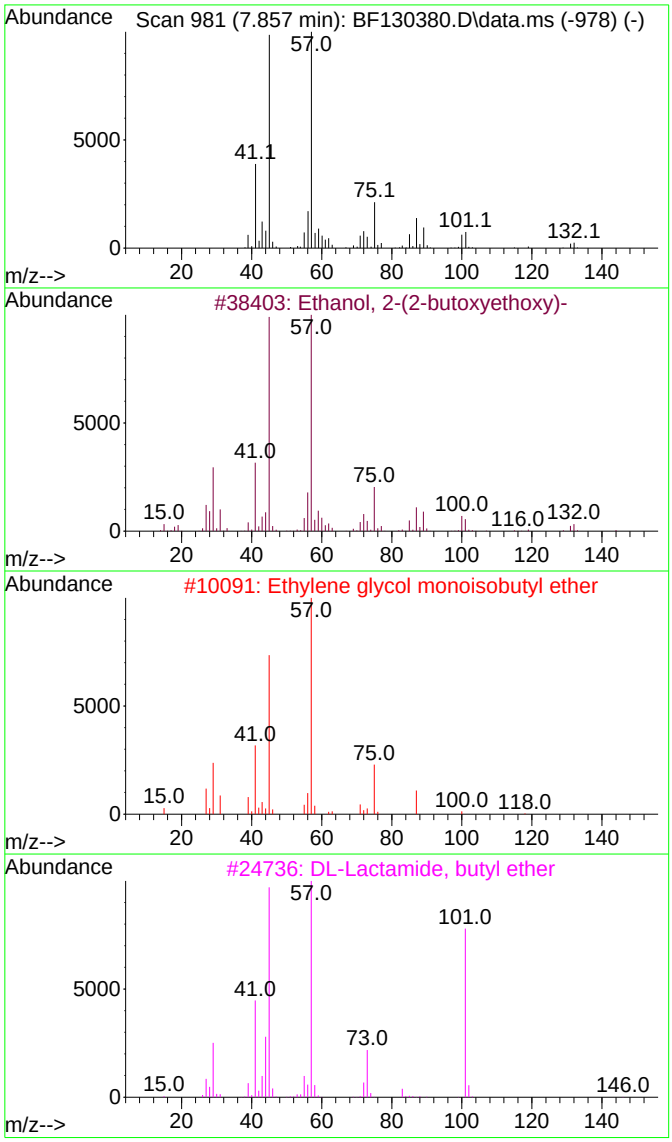
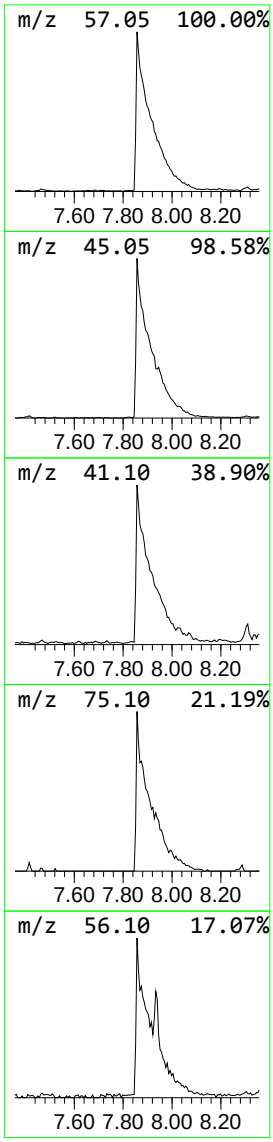
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.857	22.66 ng	951572	Naphthalene-d8	7.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
3	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	50
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





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TIC Library : C:\Database\NIST20.L
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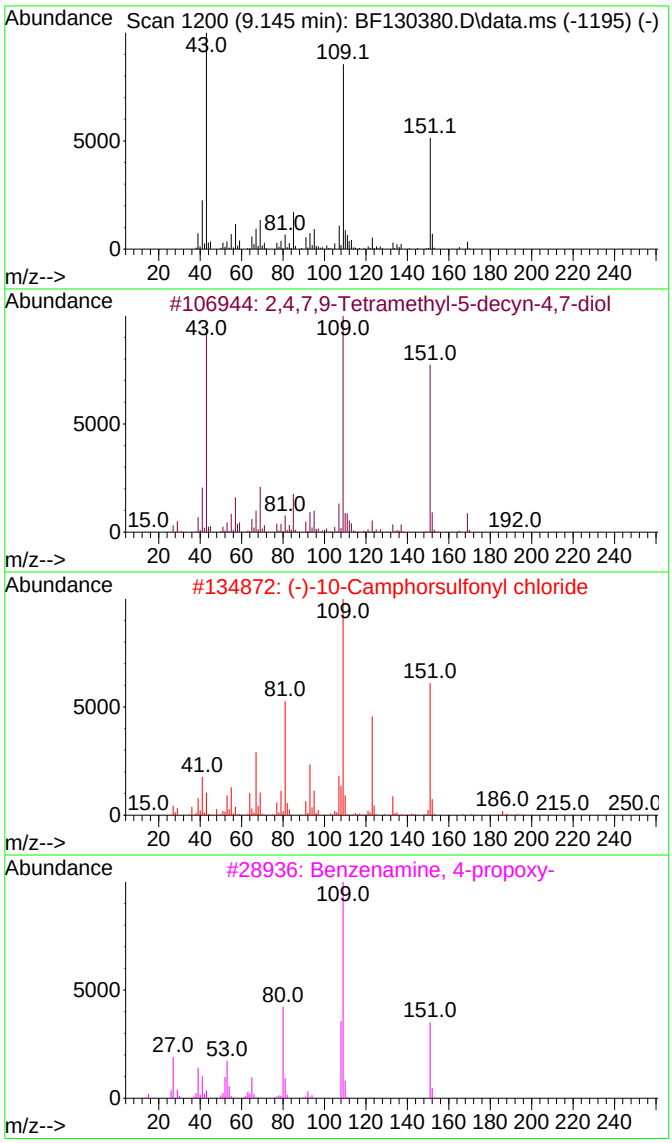
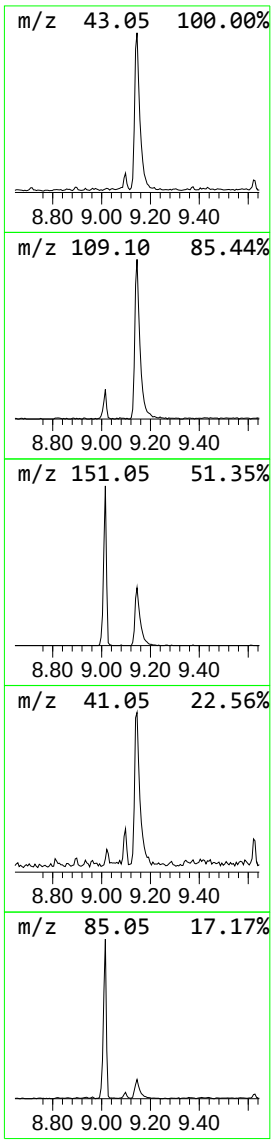
****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.145	10.32 ng	394514	Acenaphthene-d10	9.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	64
3	Benzenamine, 4-propoxy-	151	C9H13NO	004469-80-1	53
4	Metacetamol	151	C8H9NO2	000621-42-1	53
5	Acetaminophen	151	C8H9NO2	000103-90-2	53





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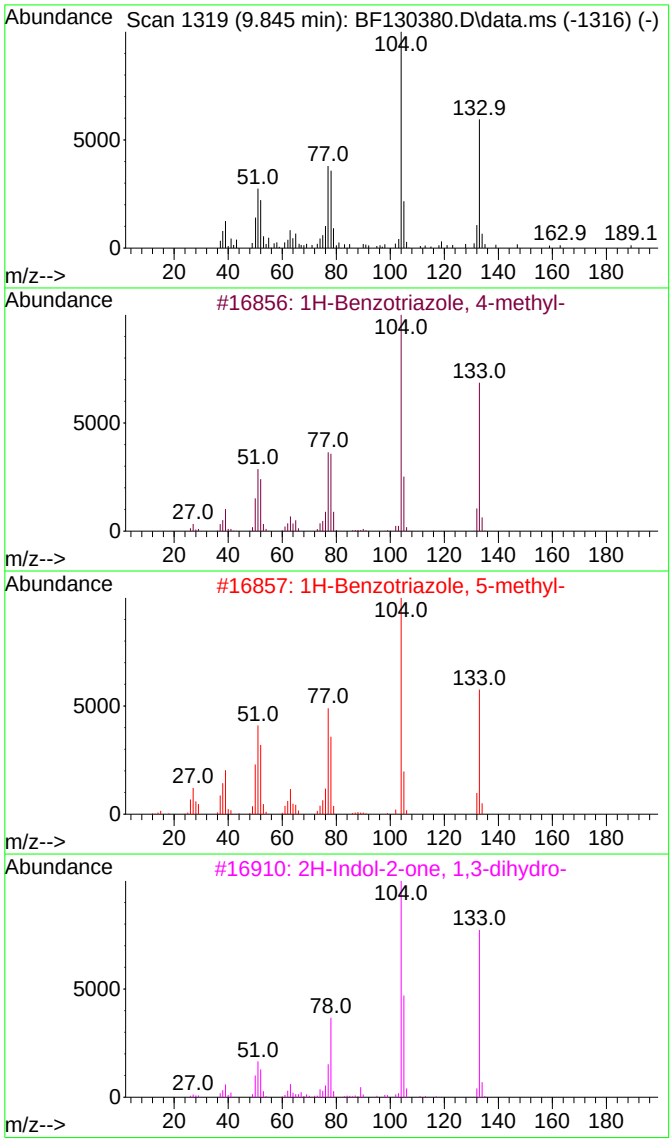
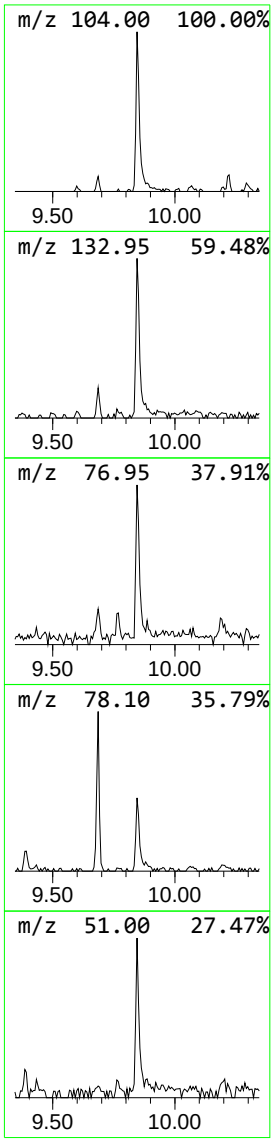
****

Peak Number 4 1H-Benzotriazole, 4-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.845	2.13 ng	81555	Acenaphthene-d10	9.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	98
2	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	97
3	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	87
4	Benzene, 1-isocyanato-2-methyl-	133	C8H7NO	000614-68-6	53
5	1H-Indol-4-ol	133	C8H7NO	002380-94-1	49





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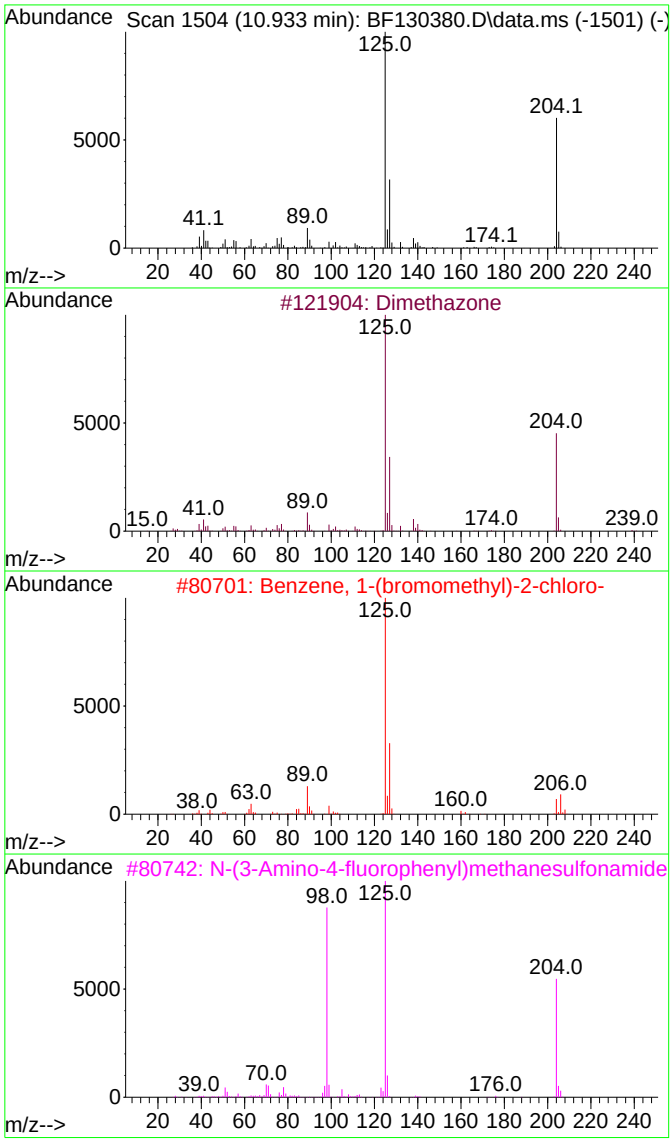
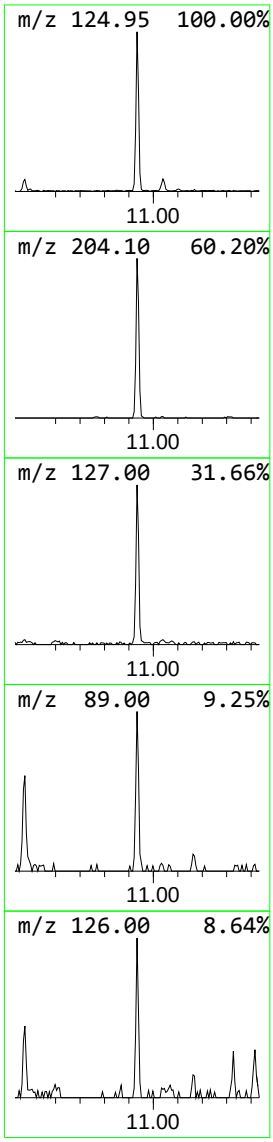
****

Peak Number 5 Dimethazone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.933	4.66 ng	144340	Phenanthrene-d10	11.168

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethazone	239	C12H14ClNO2	081777-89-1	83
2	Benzene, 1-(bromomethyl)-2-chloro-	204	C7H6BrCl	000611-17-6	64
3	N-(3-Amino-4-fluorophenyl)methan...	204	C7H9FN2O2S	926270-06-6	59
4	[(4-Chlorobenzyl)sulfonyl]acetic...	320	C12H17ClO4SSi	1000468-75-9	53
5	Diglycolic acid, 4-chlorobenzyl ...	342	C17H23ClO5	1000382-25-8	53





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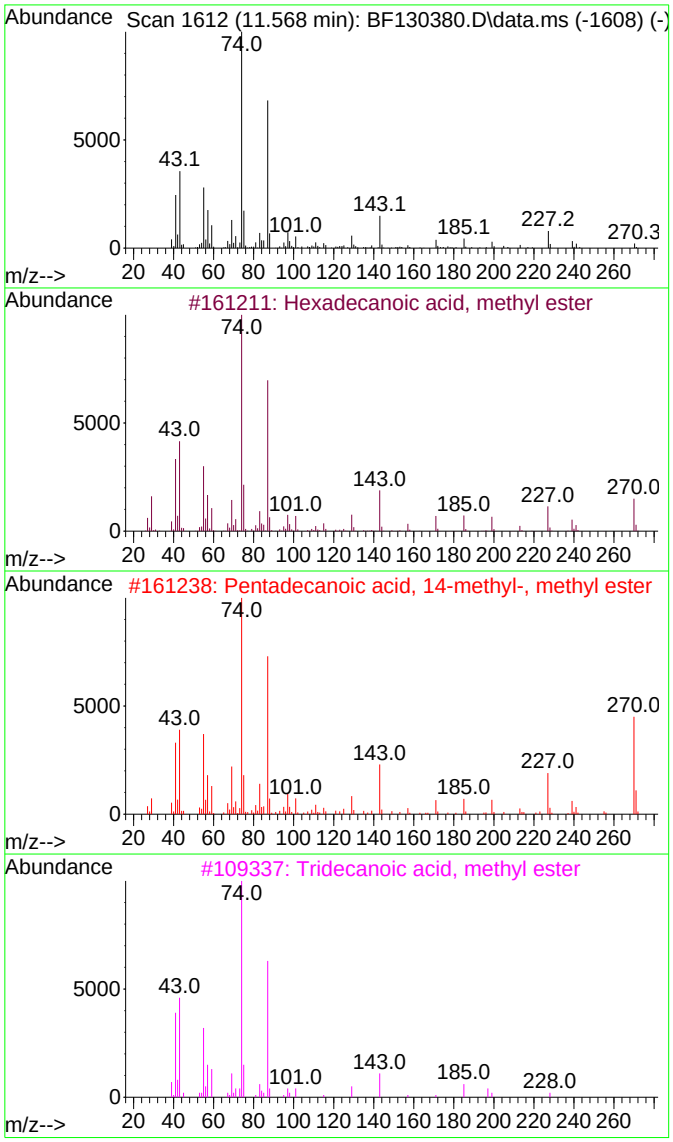
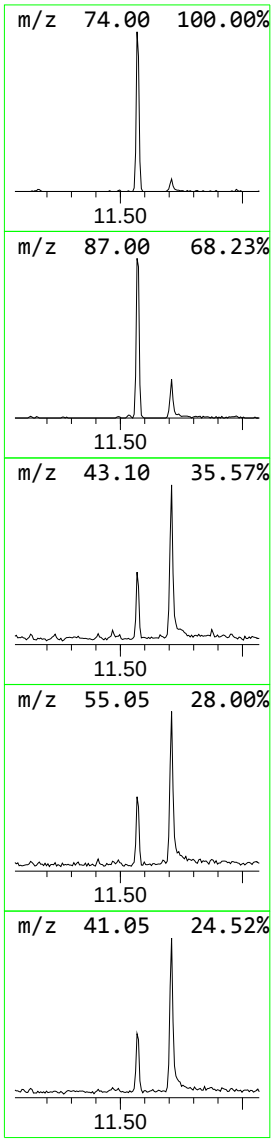
****
Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.568	6.03 ng	186776	Phenanthrene-d10	11.168

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90





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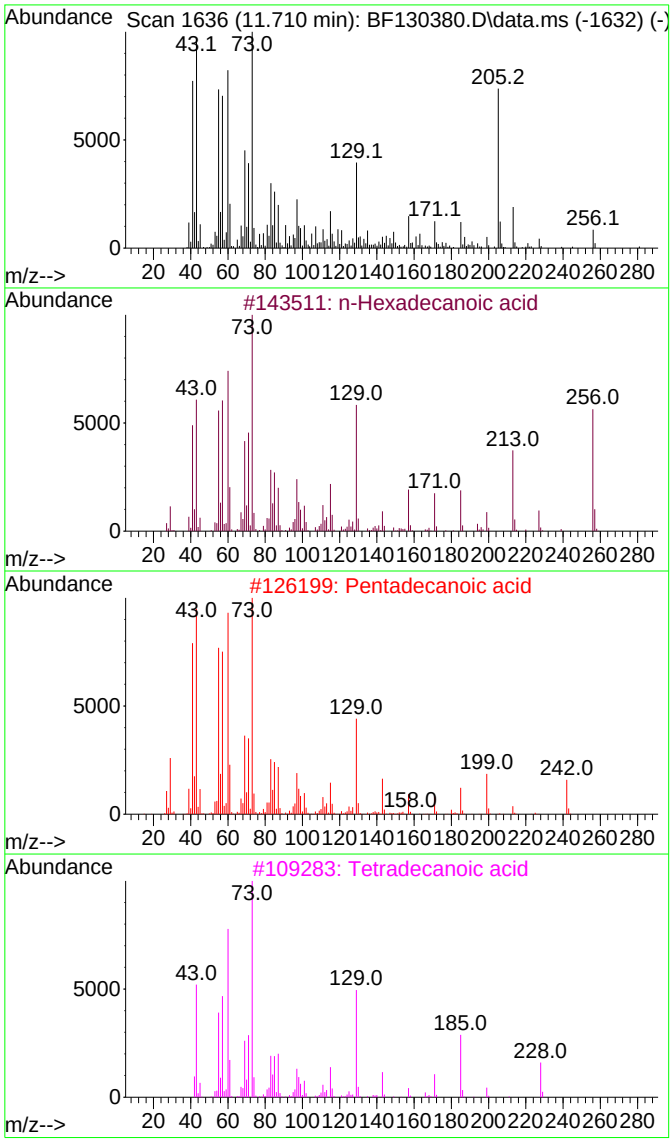
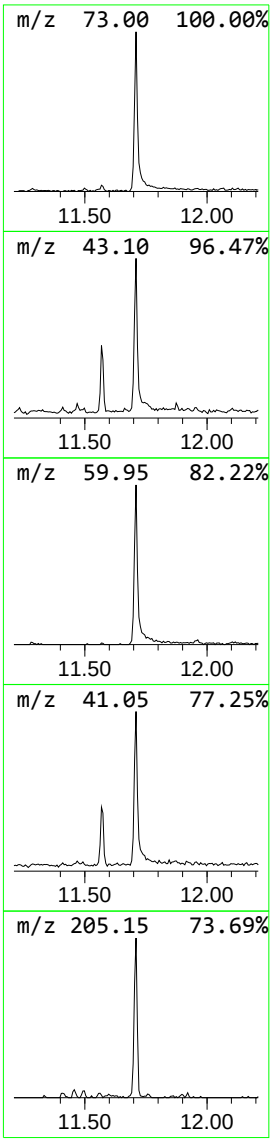
Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.710	17.16 ng	531062	Phenanthrene-d10	11.168

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	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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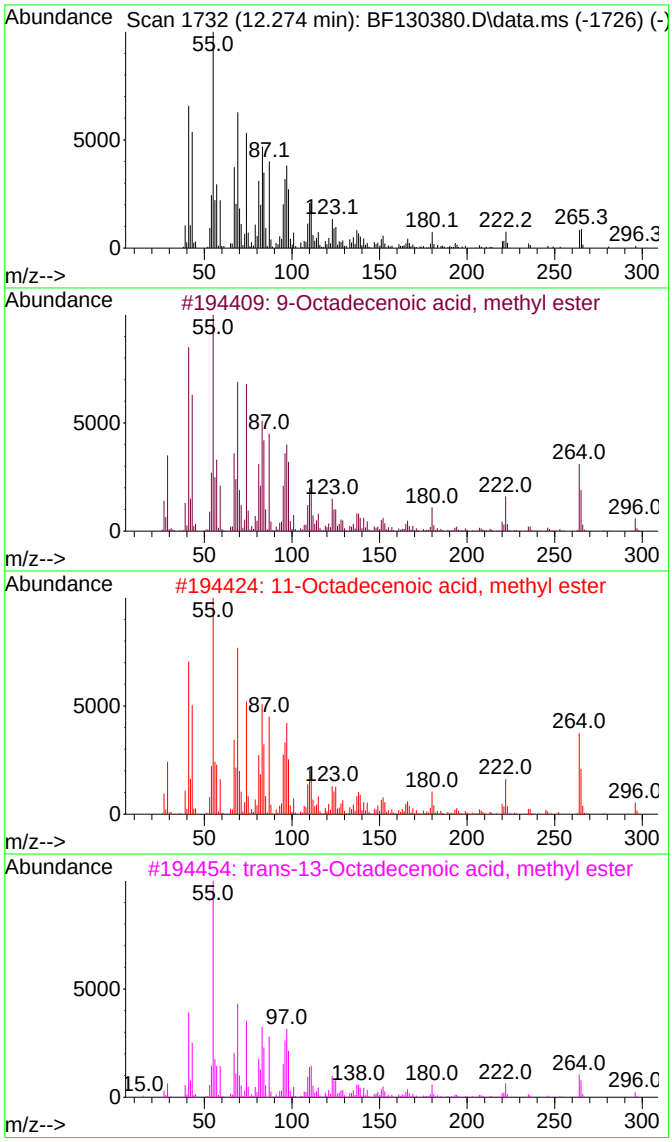
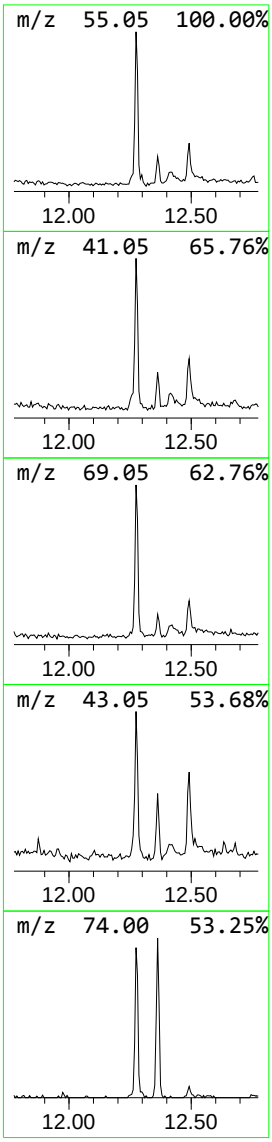
Peak Number 8 9-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.274	11.28 ng	349076	Phenanthrene-d10	11.168

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	99
4	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	99
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99





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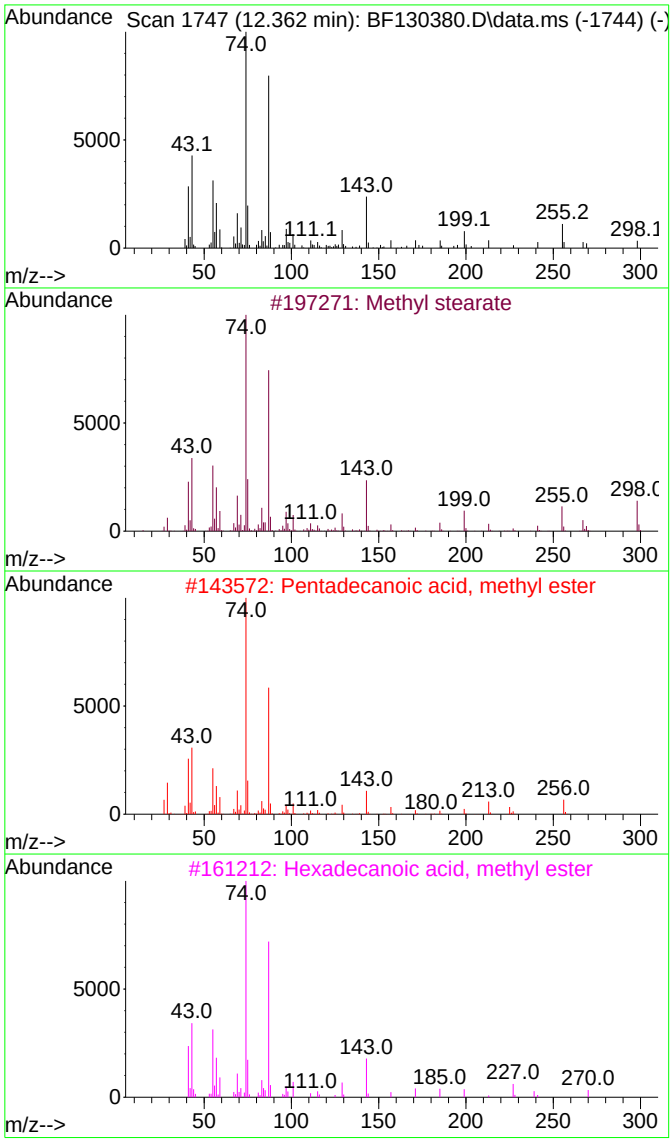
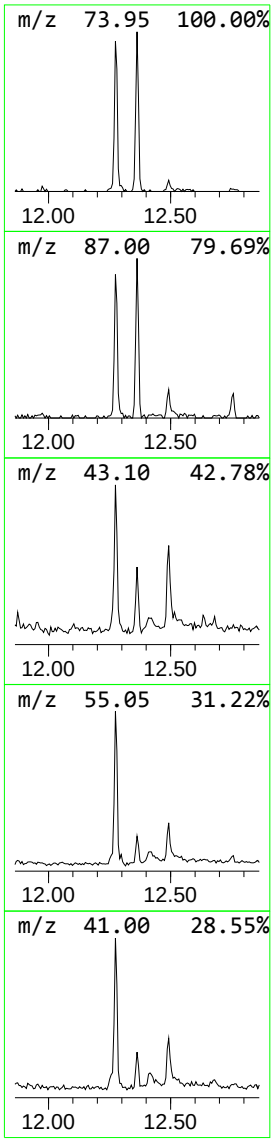
****

Peak Number 9 Methyl stearate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.363	2.30 ng	71108	Phenanthrene-d10	11.168

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
3	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	74





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Acq On : 22 Sep 2022 17:32
Operator : CG\JU
Sample : N4609-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN002

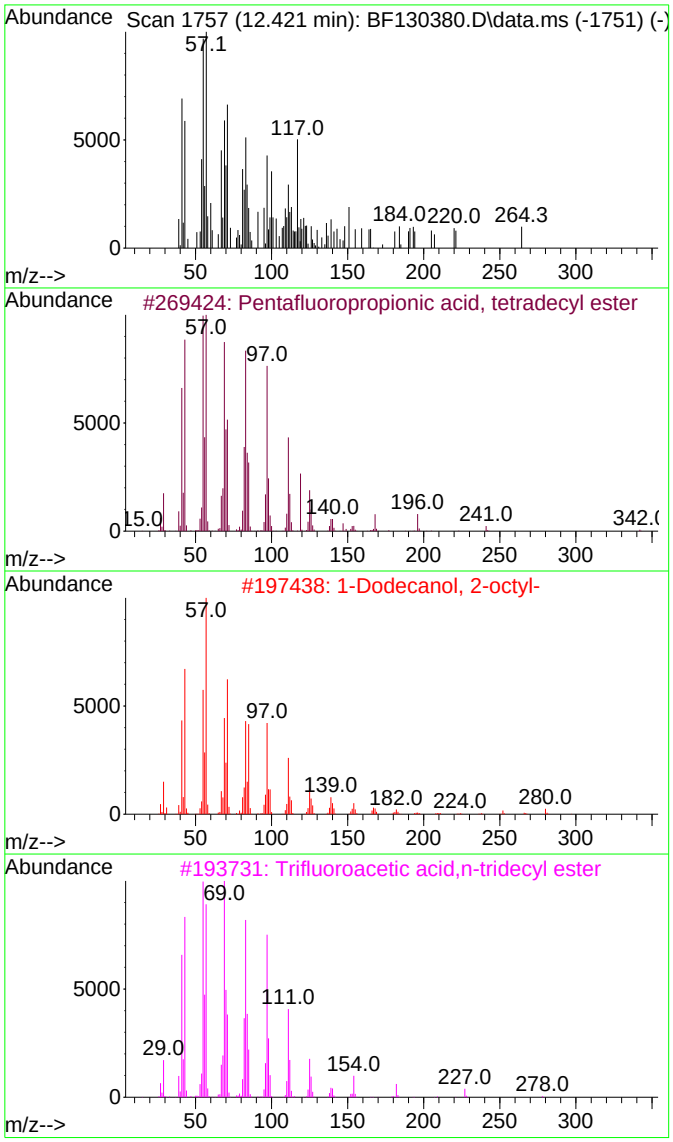
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

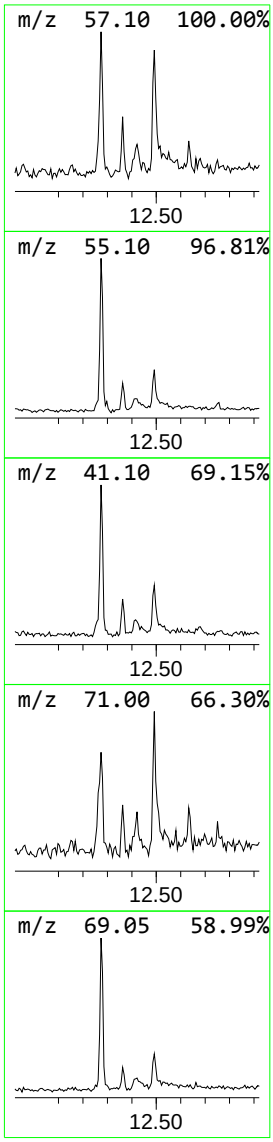
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	2.64 ng	81861	Phenanthrene-d10	11.168

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	55
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	49
3	Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	49
4	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	49
5	Hexanoic acid, heptadecyl ester	354	C23H46O2	1000282-83-9	47





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

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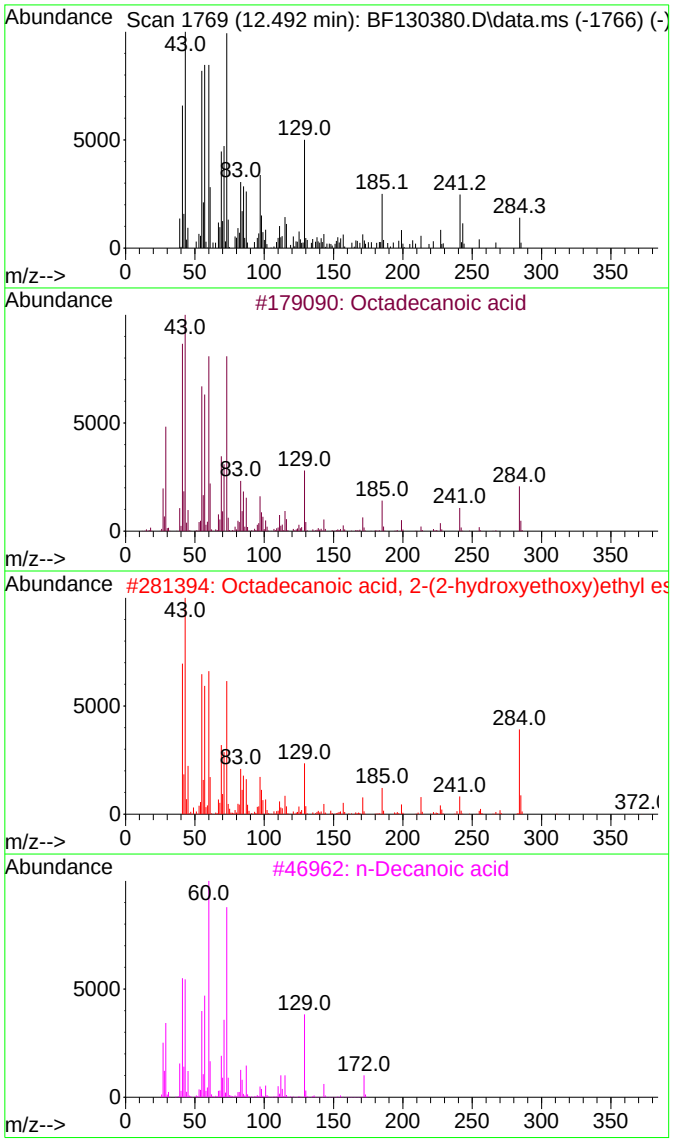
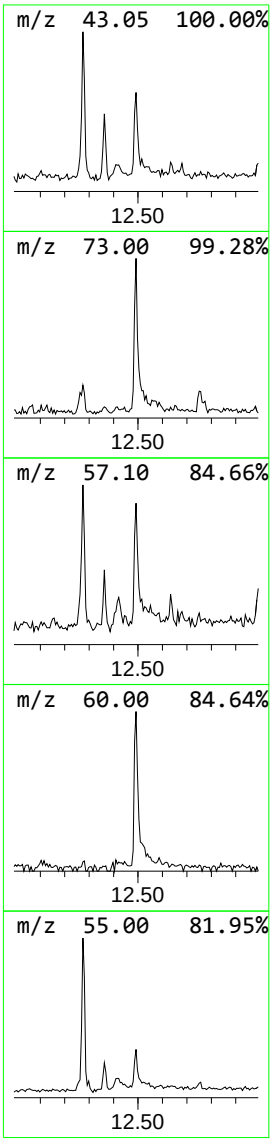
Peak Number 11 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	4.29 ng	133020	Chrysene-d12	13.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	46





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Operator : CG\JU
Sample : N4609-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN002

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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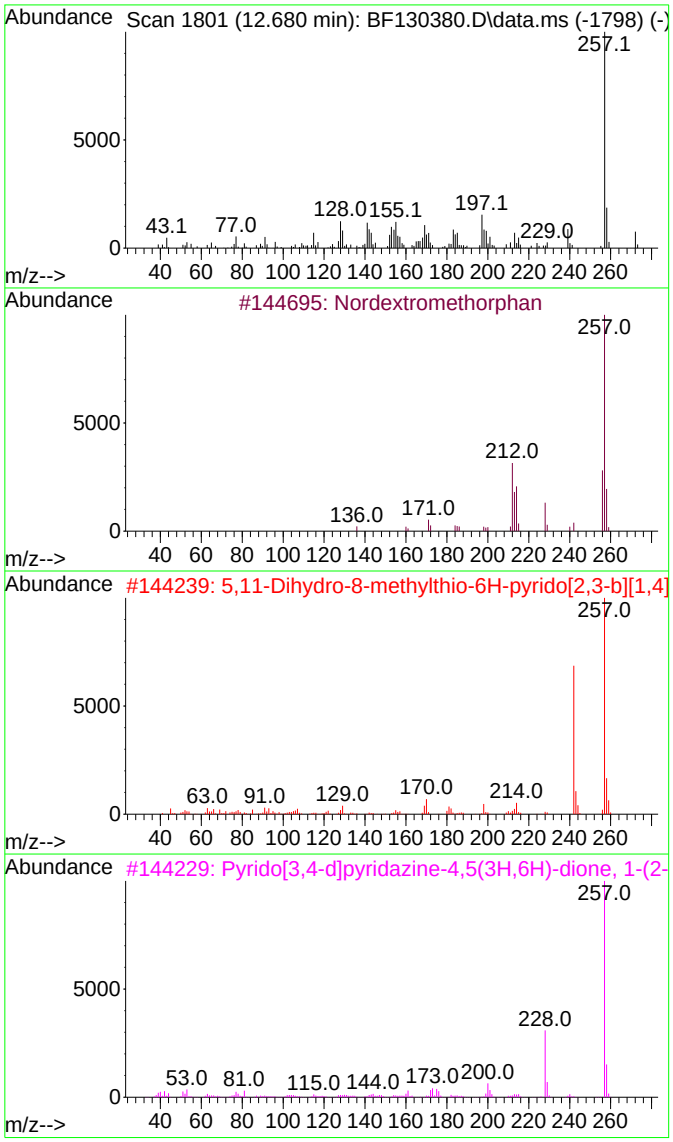
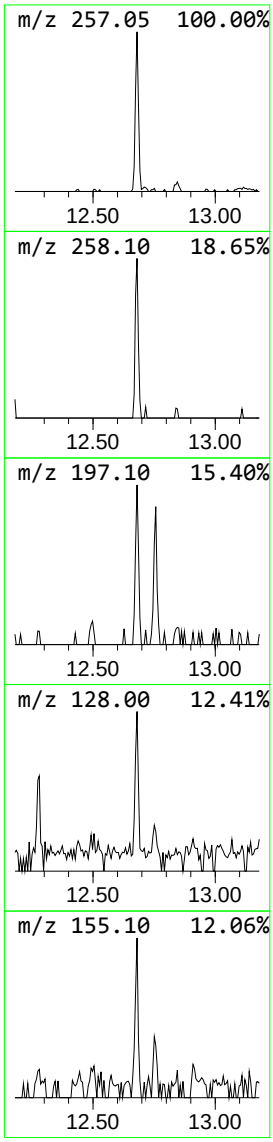
Peak Number 12 Nordextromethorphan Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	2.09 ng	64867	Chrysene-d12	13.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nordextromethorphan	257	C17H23NO	051195-74-5	64
2	5,11-Dihydro-8-methylthio-6H-pyr...	257	C13H11N3OS	133727-45-4	59
3	Pyrido[3,4-d]pyridazine-4,5(3H,6...	257	C13H11N3O3	160033-05-6	49
4	5-Hydroxyimino-4-phenylhydrazono...	257	C12H11N5O2	1000110-69-8	49
5	2-Methyl-2-p-tolyl-1-acenaphthenone	272	C20H16O	136861-27-3	47





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

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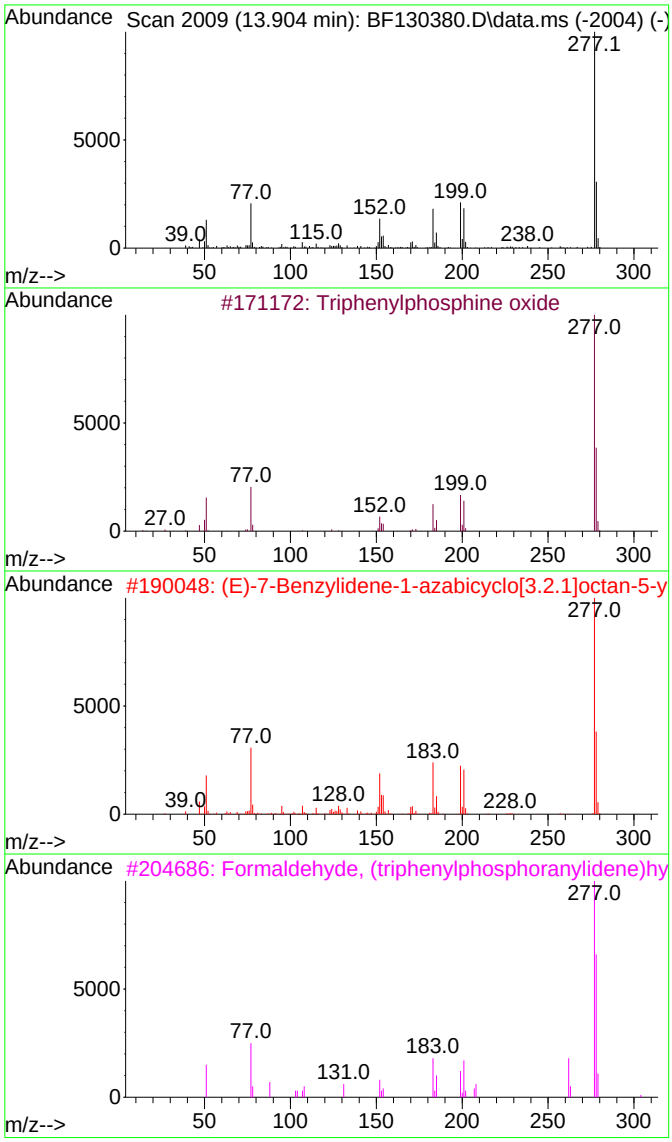
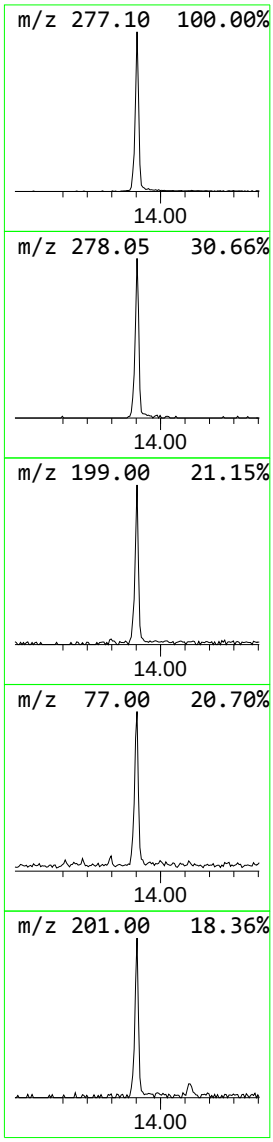
Peak Number 13 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.903	7.75 ng	240568	Chrysene-d12	13.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	87
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	40
5	1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	32





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Misc :
ALS Vial : 9 Sample Multiplier: 1

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

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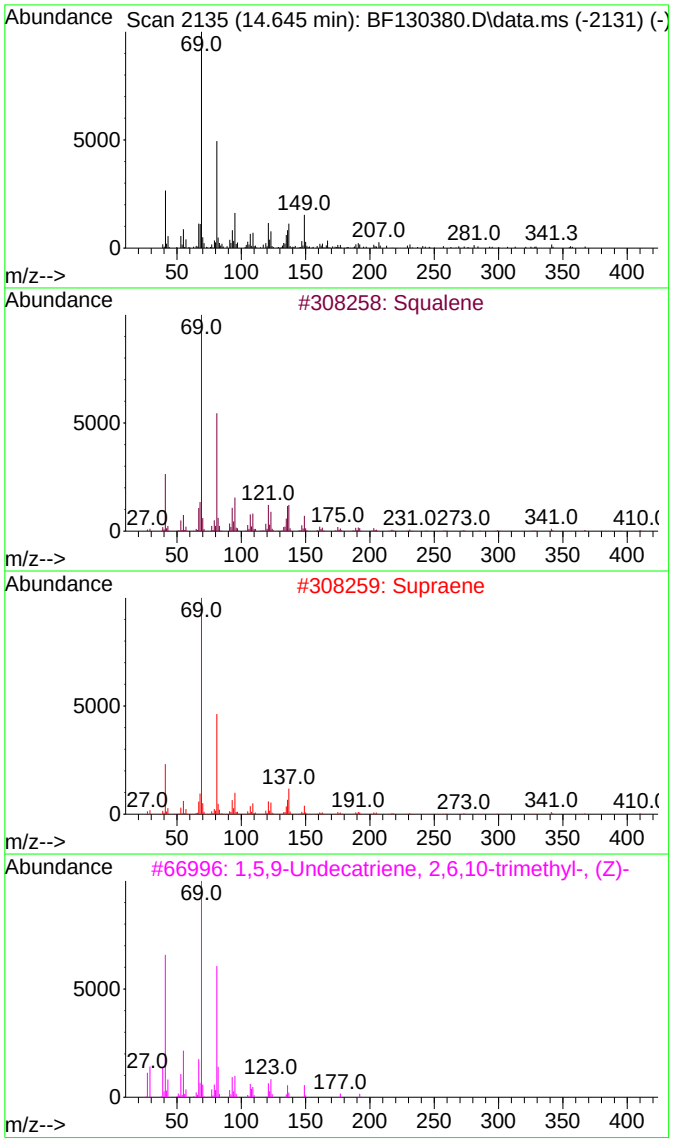
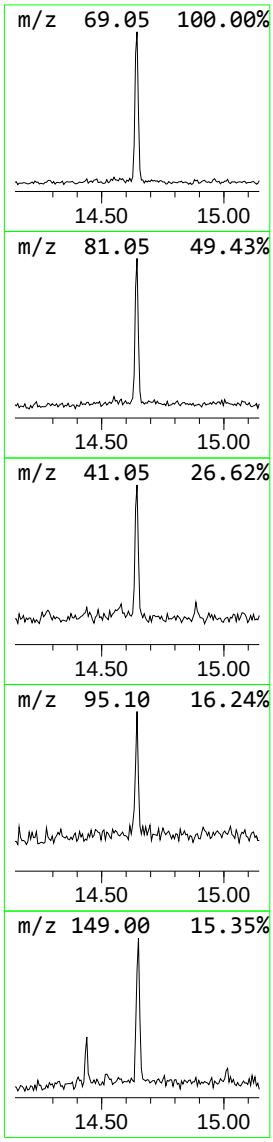
Peak Number 14 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.645	5.04 ng	137843	Perylene-d12	15.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	80
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	68
4	Farnesol isomer a	222	C15H26O	1000108-92-4	59
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	53





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
2-Pentanone, 4-...	4.834	3.5	ng	112464	1	6.657	638088	20.0
Ethanol, 2-(2-b...	7.857	22.7	ng	951572	2	7.939	839762	20.0
2,4,7,9-Tetrame...	9.145	10.3	ng	394514	3	9.686	764468	20.0
1H-Benzotriazol...	9.845	2.1	ng	81555	3	9.686	764468	20.0
Dimethazone	10.933	4.7	ng	144340	4	11.168	619050	20.0
Hexadecanoic ac...	11.568	6.0	ng	186776	4	11.168	619050	20.0
n-Hexadecanoic ...	11.710	17.2	ng	531062	4	11.168	619050	20.0
9-Octadecenoic ...	12.274	11.3	ng	349076	4	11.168	619050	20.0
Methyl stearate	12.363	2.3	ng	71108	4	11.168	619050	20.0
Pentafluoroprop...	12.421	2.6	ng	81861	4	11.168	619050	20.0
Octadecanoic acid	12.492	4.3	ng	133020	5	13.798	620420	20.0
Nordextromethor...	12.680	2.1	ng	64867	5	13.798	620420	20.0
Triphenylphosph...	13.903	7.8	ng	240568	5	13.798	620420	20.0
Squalene	14.645	5.0	ng	137843	6	15.192	546707	20.0