

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072922\
 Data File : BF129446.D
 Acq On : 29 Jul 2022 17:31
 Operator : CG\JU
 Sample : N3969-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHAMBERS-STREET-A3-9065X-MH

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-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.104	476	479	485	rVB	76785	76958	1.74%	0.348%
2	5.522	546	550	558	rBV	1096149	1068232	24.13%	4.830%
3	6.528	718	721	729	rVB	742130	653890	14.77%	2.956%
4	6.881	778	781	785	rBV	1173198	975248	22.03%	4.409%
5	7.451	871	878	881	rBV	2563166	2474360	55.90%	11.187%
6	8.169	995	1000	1003	rBV	1508047	1293979	29.23%	5.851%
7	9.245	1177	1183	1186	rBV	5069921	4426496	100.00%	20.014%
8	9.357	1198	1202	1205	rBV	71276	65262	1.47%	0.295%
9	9.928	1295	1299	1302	rBV	1622883	1398838	31.60%	6.325%
10	10.128	1326	1333	1341	rBV	290474	486677	10.99%	2.200%
11	10.716	1430	1433	1437	rBV	1627742	1506387	34.03%	6.811%
12	10.969	1473	1476	1478	rBV2	52276	69749	1.58%	0.315%
13	10.992	1478	1480	1487	rVB	83906	112025	2.53%	0.507%
14	11.075	1488	1494	1499	rBV3	88701	156924	3.55%	0.710%
15	11.416	1548	1552	1556	rBV	1434562	1167087	26.37%	5.277%
16	11.645	1587	1591	1596	rBV3	96656	143746	3.25%	0.650%
17	11.798	1613	1617	1620	rBV	235158	208326	4.71%	0.942%
18	11.933	1637	1640	1642	rBV2	95514	93379	2.11%	0.422%
19	12.463	1727	1730	1734	rBV2	134180	220163	4.97%	0.995%
20	12.504	1734	1737	1740	rVB	585819	467309	10.56%	2.113%
21	12.586	1749	1751	1755	rBV	129406	112358	2.54%	0.508%
22	12.651	1759	1762	1765	rVB2	185906	152516	3.45%	0.690%
23	13.004	1818	1822	1825	rBV	3342817	2832952	64.00%	12.809%
24	13.904	1972	1975	1984	rVB4	101980	164008	3.71%	0.742%
25	14.063	1998	2002	2006	rBV	989542	814058	18.39%	3.681%
26	15.557	2252	2256	2264	rVB	773980	976346	22.06%	4.414%

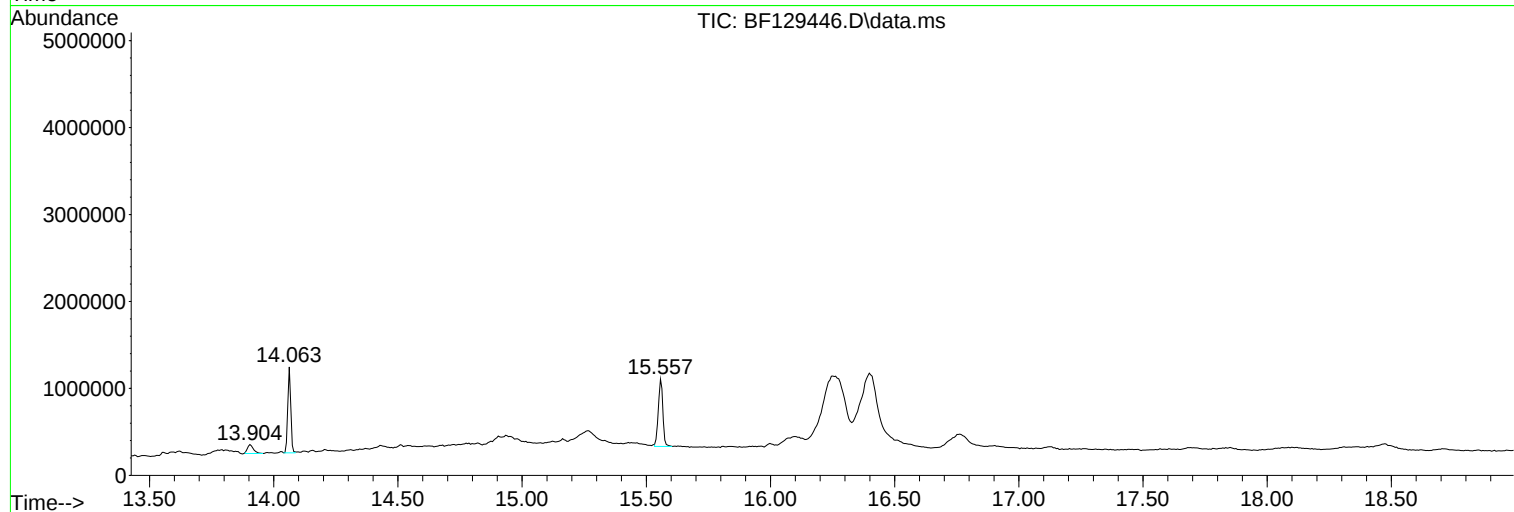
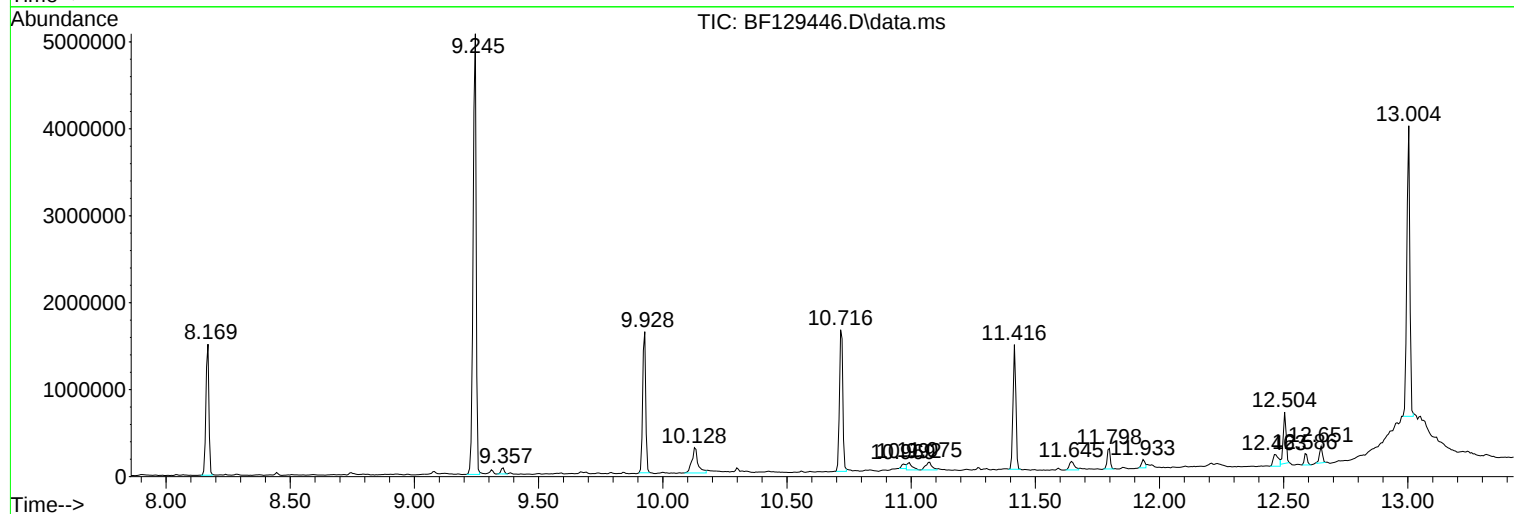
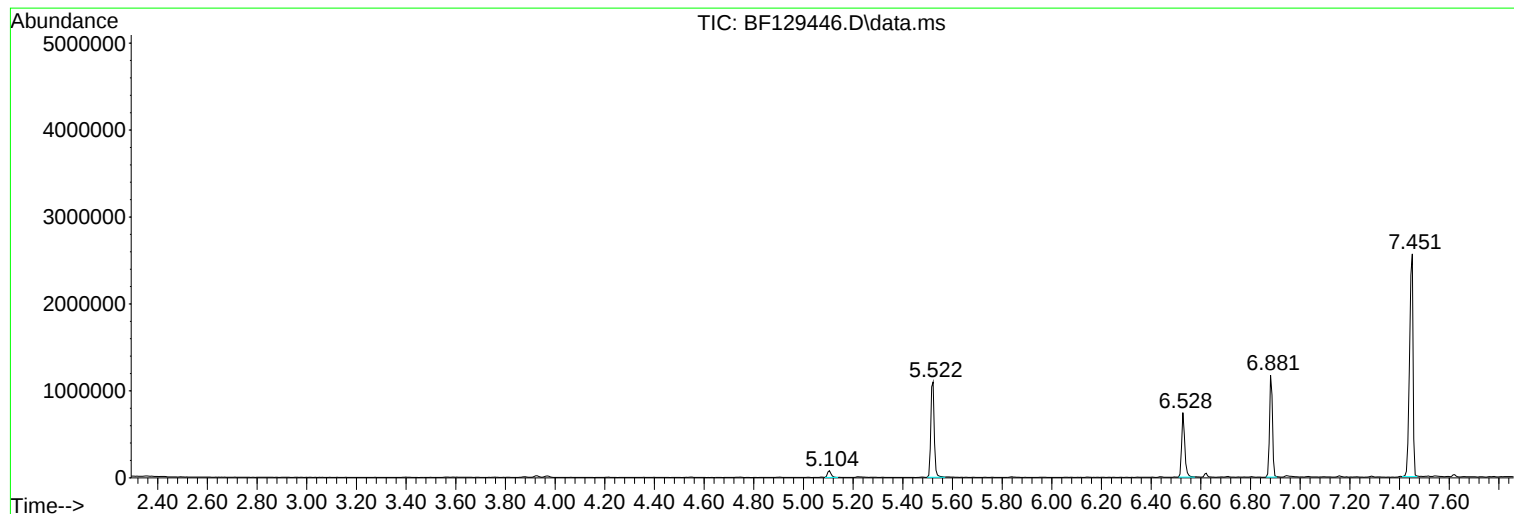
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CHAMBERS-STREET-A3-9065X-MH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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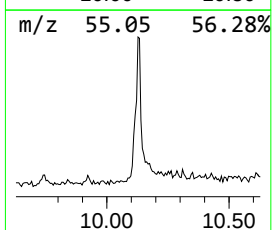
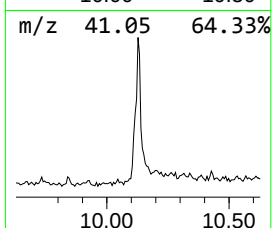
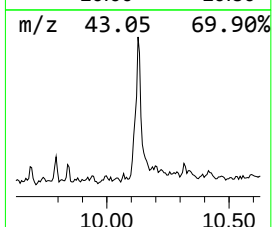
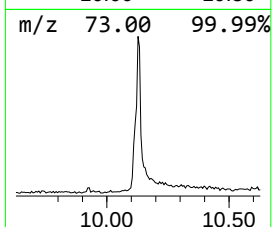
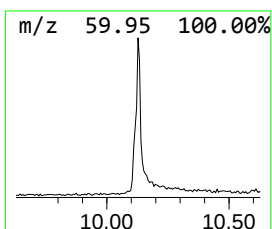
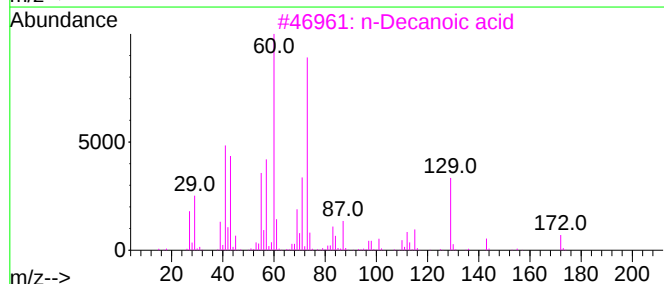
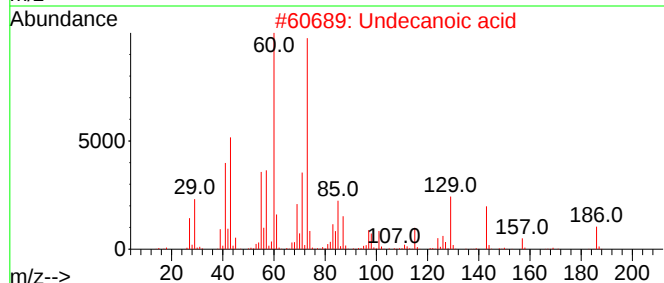
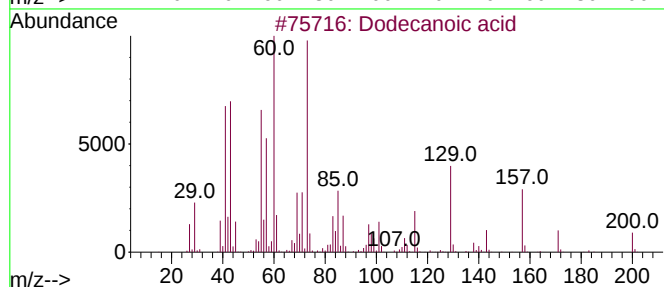
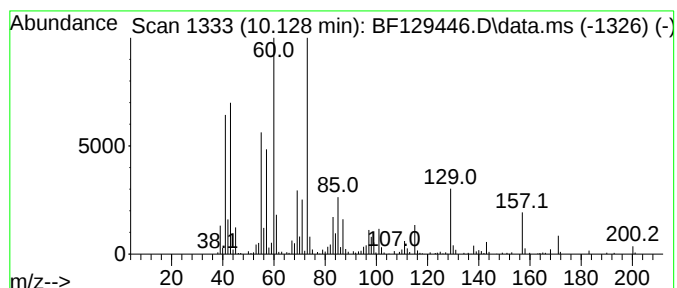
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Dodecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.128	6.96 ng	486677	Acenaphthene-d10	9.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	98
2			Undecanoic acid	186	C11H22O2	000112-37-8	80
3			n-Decanoic acid	172	C10H20O2	000334-48-5	70
4			Nonanoic acid	158	C9H18O2	000112-05-0	64
5			Octanoic acid	144	C8H16O2	000124-07-2	47



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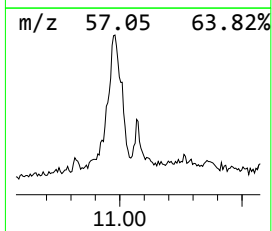
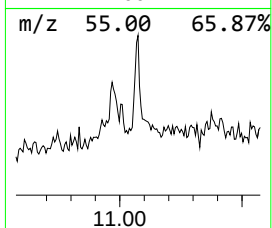
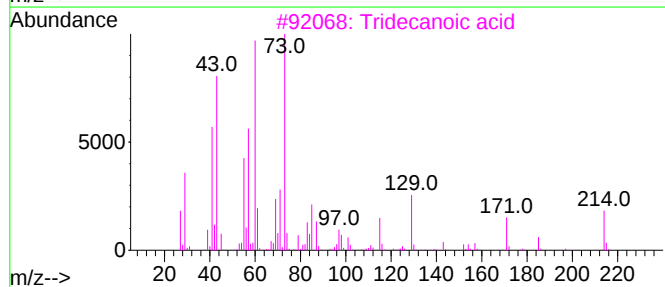
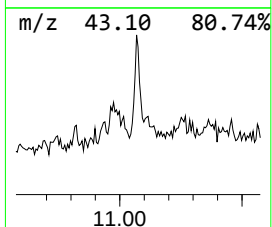
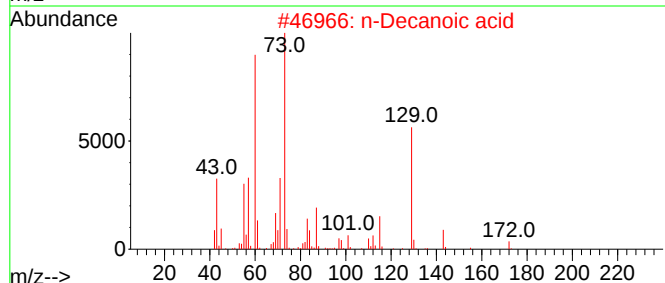
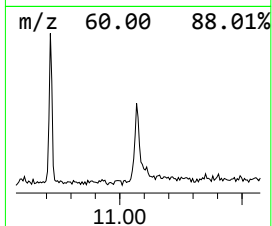
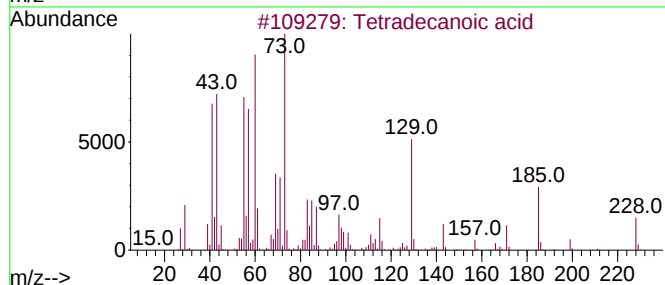
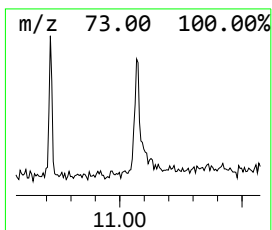
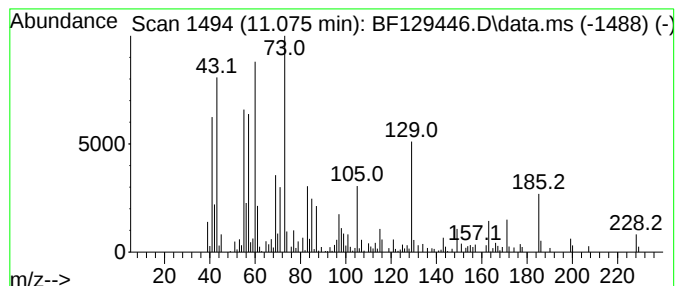
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Peak Number 2 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.075	2.69 ng	156924	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
2			n-Decanoic acid	172	C10H20O2	000334-48-5	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	59
4			Dodecanoic acid	200	C12H24O2	000143-07-7	50
5			Undecanoic acid	186	C11H22O2	000112-37-8	27



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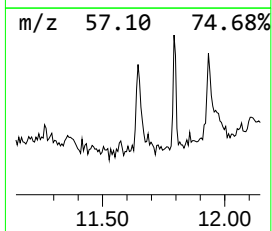
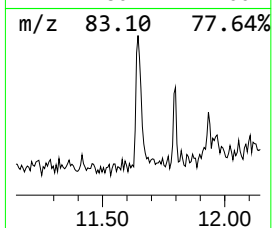
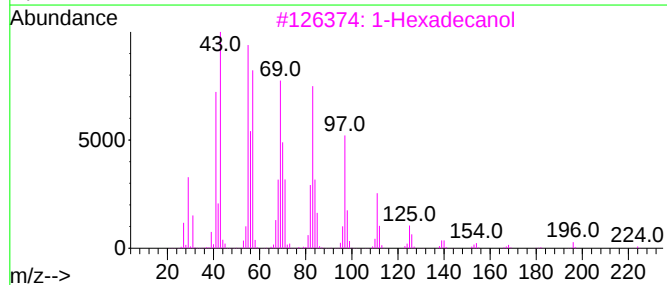
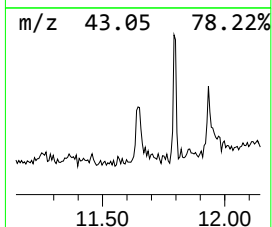
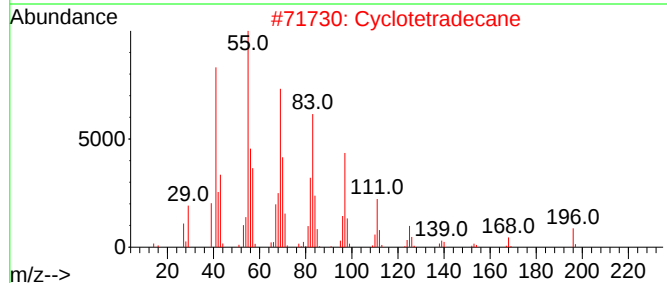
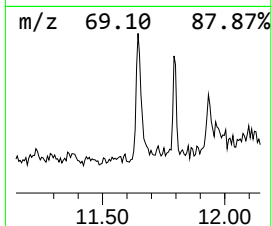
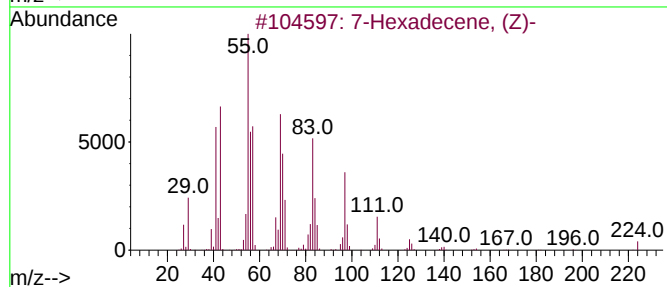
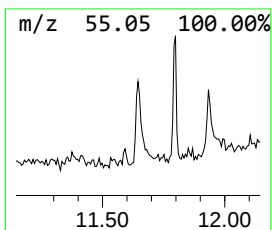
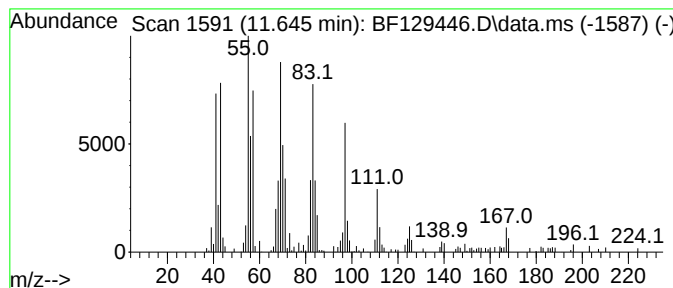
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BNA_F
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CHAMBERS-STREET-A3-9065X-MH

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

Peak Number 3 7-Hexadecene, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.645	2.46 ng	143746	Phenanthrene-d10	11.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	95
2	Cyclotetradecane	196	C14H28	000295-17-0	95
3	1-Hexadecanol	242	C16H34O	036653-82-4	95
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	94
5	1-Octadecanol	270	C18H38O	000112-92-5	94



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Misc :
ALS Vial : 5 Sample Multiplier: 1

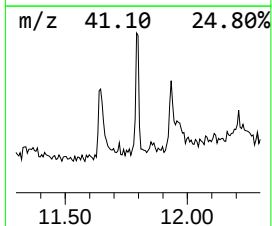
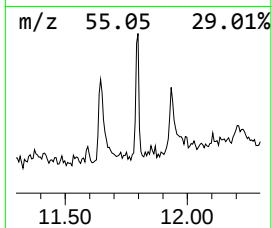
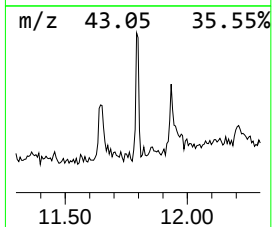
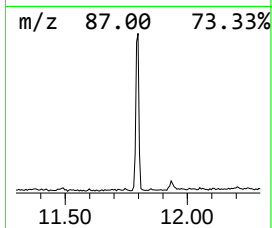
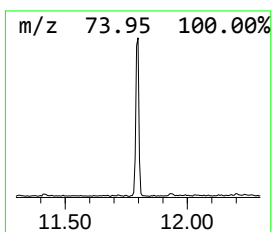
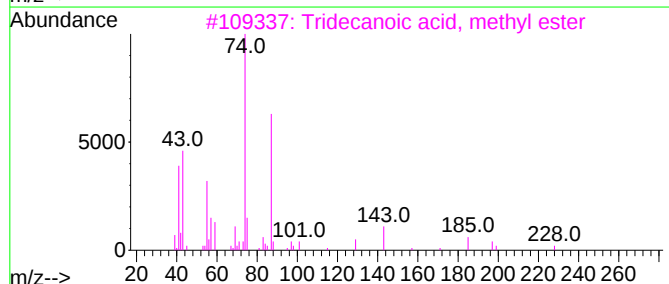
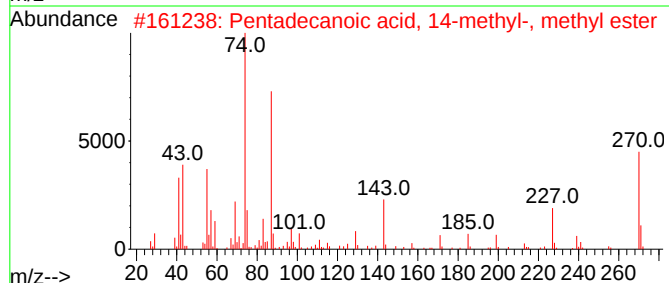
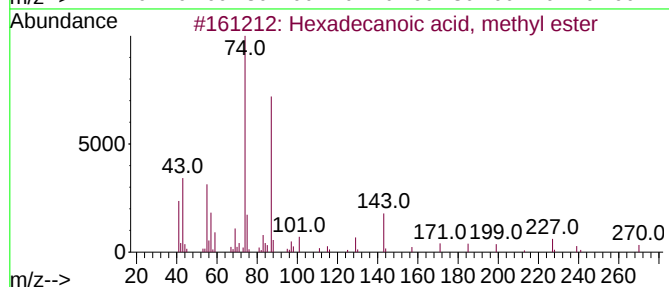
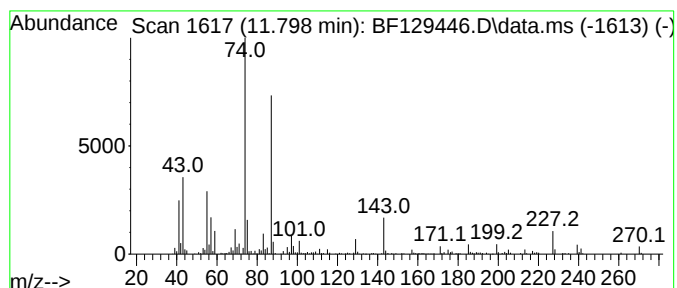
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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.798	3.57 ng	208326	Phenanthrene-d10	11.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	92
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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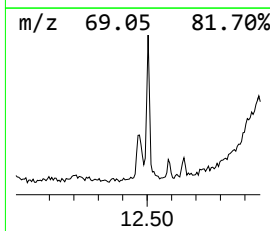
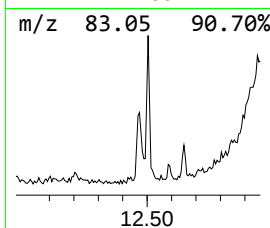
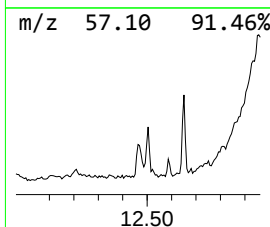
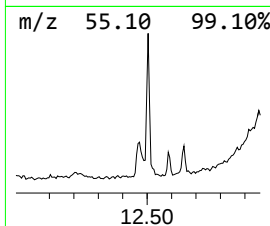
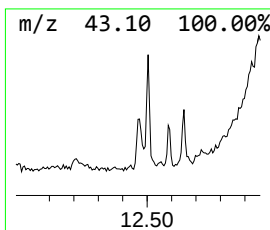
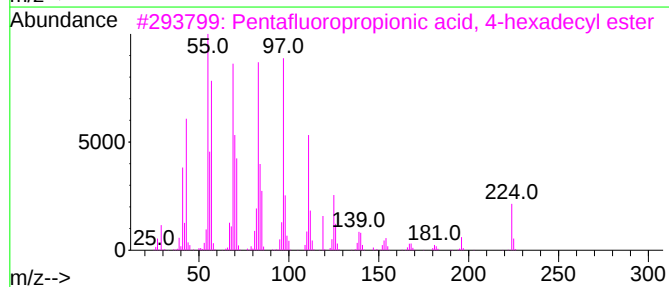
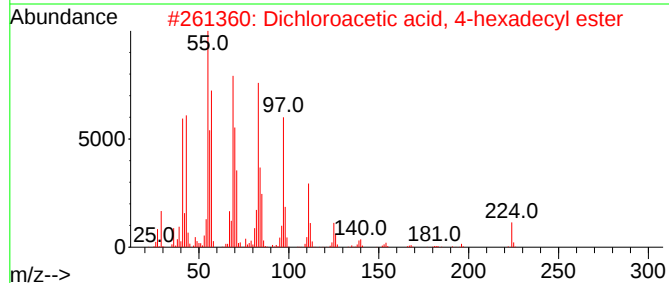
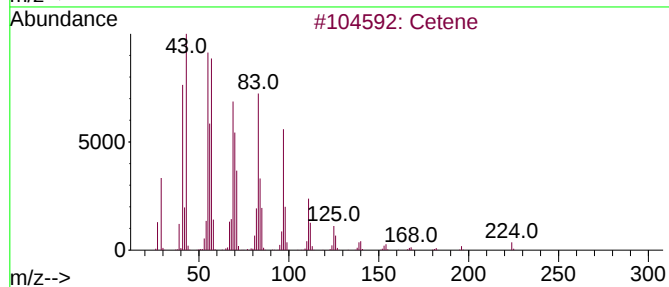
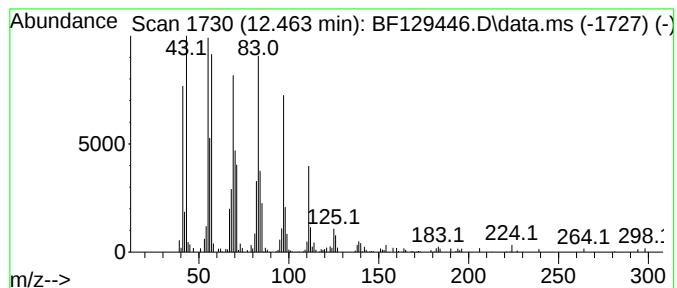
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Peak Number 5 Cetene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	3.77 ng	220163	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cetene	224	C16H32	000629-73-2	99
2			Dichloroacetic acid, 4-hexadecyl...	352	C18H34Cl2O2	1000282-98-1	94
3			Pentafluoropropionic acid, 4-hex...	388	C19H33F5O2	1000283-04-1	91
4			1-Nonadecene	266	C19H38	018435-45-5	91
5			Cyclohexadecane	224	C16H32	000295-65-8	91



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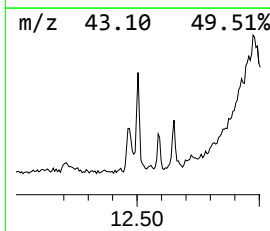
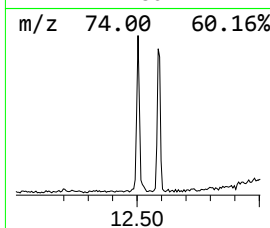
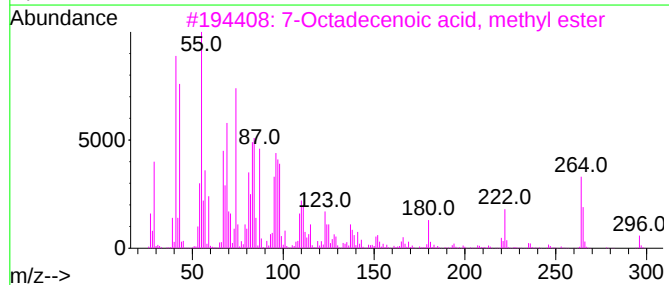
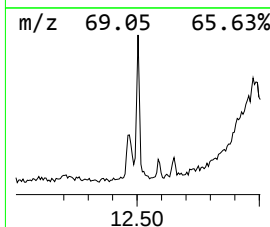
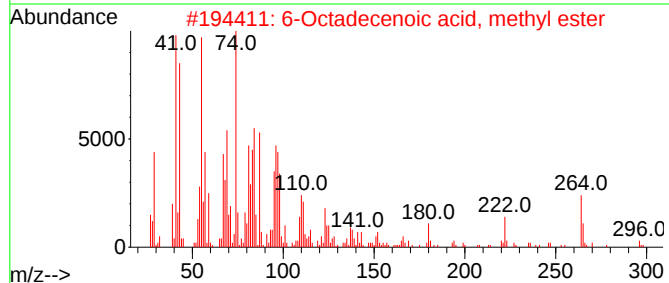
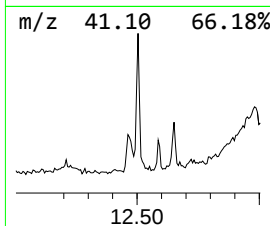
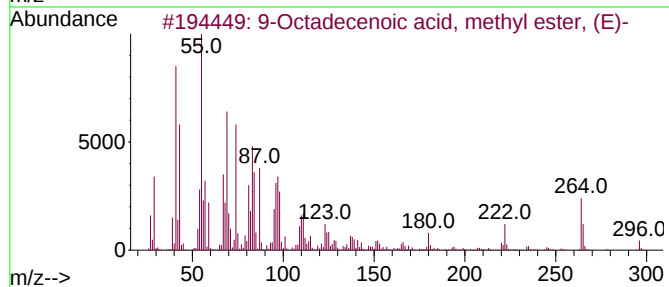
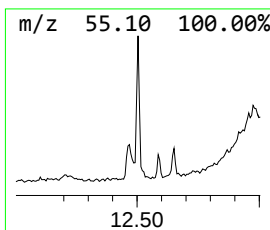
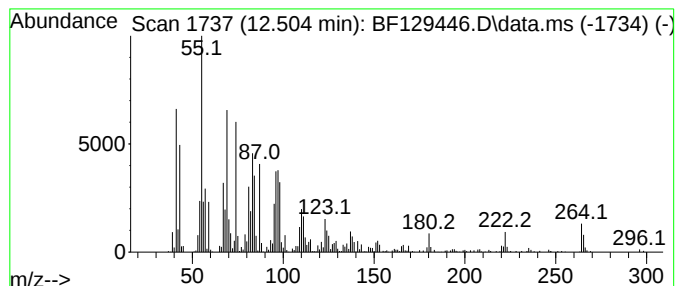
Instrument :
BNA_F
ClientSampleId :
CHAMBERS-STREET-A3-9065X-MH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.504	8.01 ng	467309	Phenanthrene-d10	11.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
2	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
3	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	99
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
5	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072922\
Data File : BF129446.D
Acq On : 29 Jul 2022 17:31
Operator : CG\JU
Sample : N3969-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

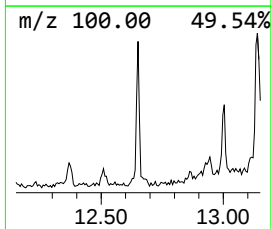
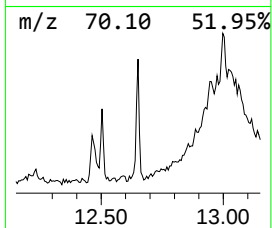
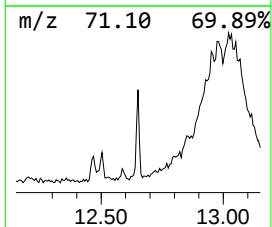
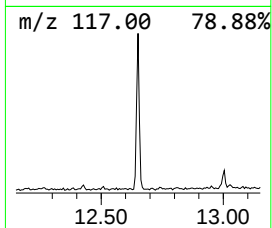
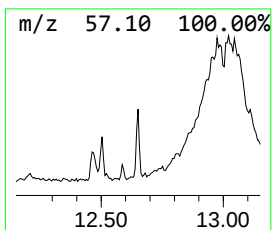
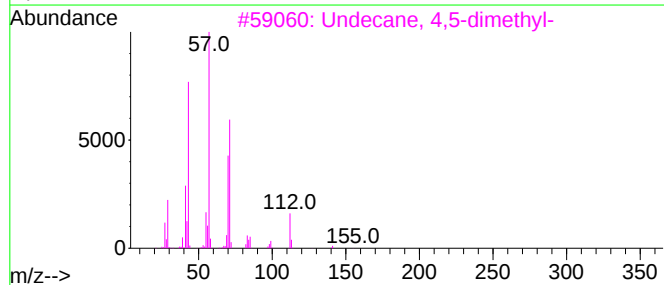
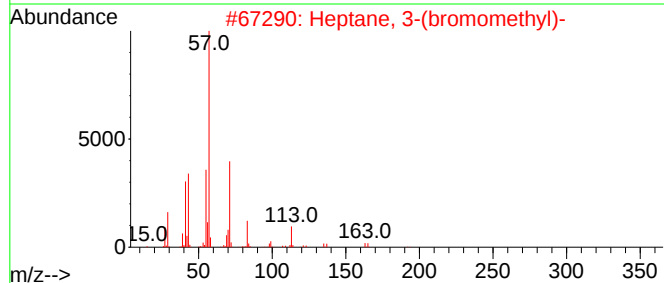
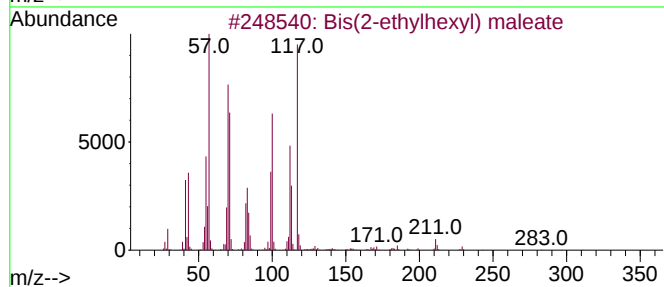
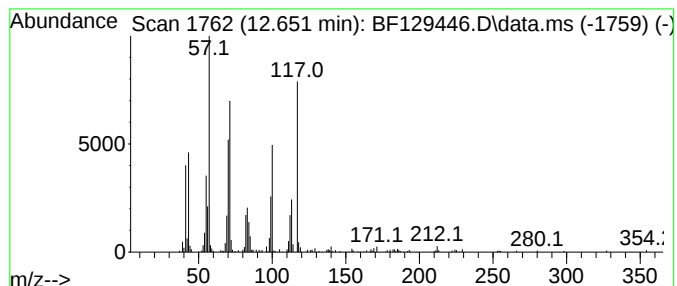
Instrument :
BNA_F
ClientSampleId :
CHAMBERS-STREET-A3-9065X-MH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.651 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.651	2.61 ng	152516	Phenanthrene-d10			11.416
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) maleate		340	C20H36O4	000142-16-5	90
2	Heptane, 3-(bromomethyl)-		192	C8H17Br	018908-66-2	22
3	Undecane, 4,5-dimethyl-		184	C13H28	017312-79-7	22
4	Sulfurous acid, 2-ethylhexyl oct...		446	C26H54O3S	1000309-20-1	22
5	Carbonic acid, propargyl 2-ethyl...		212	C12H20O3	1000357-90-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072922\
Data File : BF129446.D
Acq On : 29 Jul 2022 17:31
Operator : CG\JU
Sample : N3969-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

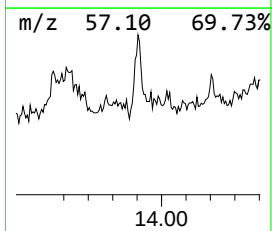
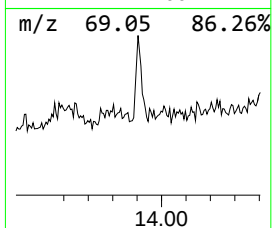
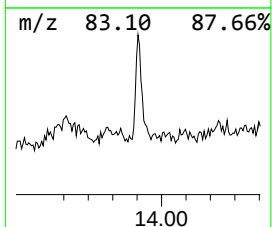
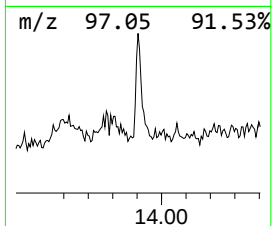
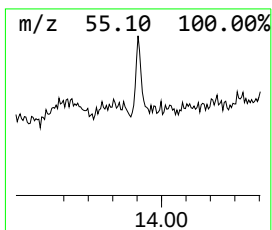
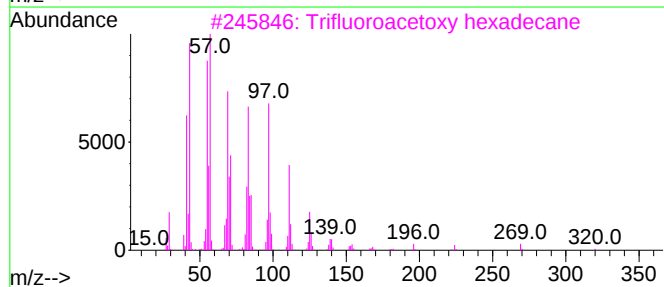
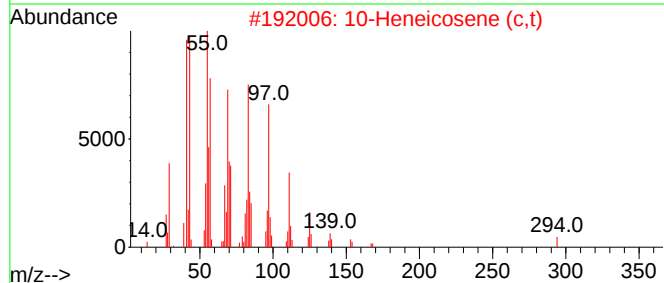
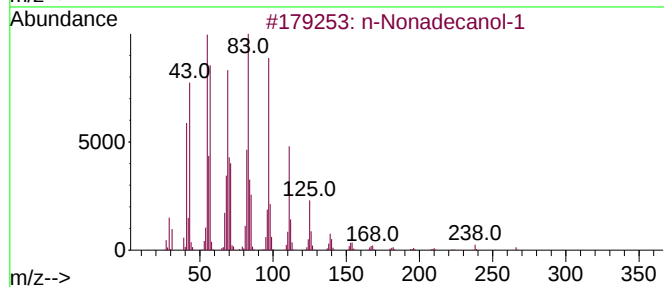
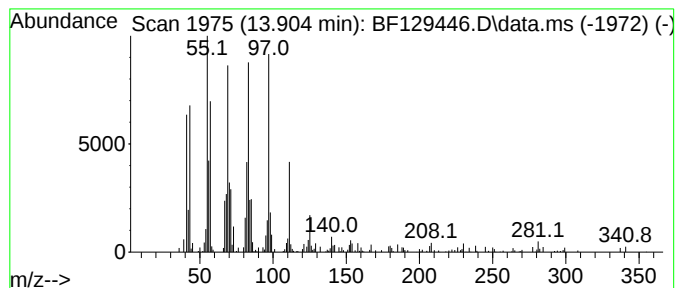
Instrument :
BNA_F
ClientSampleId :
CHAMBERS-STREET-A3-9065X-MH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.904	4.03 ng	164008	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	10-Heneicosene (c,t)	294	C21H42	095008-11-0	90
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	86
4	Cycloeicosane	280	C20H40	000296-56-0	78
5	1-Octadecanol	270	C18H38O	000112-92-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072922\
Data File : BF129446.D
Acq On : 29 Jul 2022 17:31
Operator : CG\JU
Sample : N3969-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHAMBERS-STREET-A3-9065X-MH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dodecanoic acid	10.128	7.0	ng	486677	3	9.928	1398840	20.0
Tetradecanoic acid	11.075	2.7	ng	156924	4	11.416	1167090	20.0
7-Hexadecene, (Z)-	11.645	2.5	ng	143746	4	11.416	1167090	20.0
Hexadecanoic ac...	11.798	3.6	ng	208326	4	11.416	1167090	20.0
Cetene	12.463	3.8	ng	220163	4	11.416	1167090	20.0
9-Octadecenoic ...	12.504	8.0	ng	467309	4	11.416	1167090	20.0
unknown12.651	12.651	2.6	ng	152516	4	11.416	1167090	20.0
n-Nonadecanol-1	13.904	4.0	ng	164008	5	14.063	814058	20.0