LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127093.D
Acq On : 28 Feb 2022 12:02
Operator : CG\JU
Sample : N1664-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127093.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.475	26	32	39	rVB	56850	81568	2.73%	0.370%
2	4.928	445	449	453	rBV	38902	40014	1.34%	0.182%
3	5.134	478	484	492	rVB	48558	60834	2.03%	0.276%
4	5.528	546	551	554	rBV	2662026	2406475	80.49%	10.918%
5	6.528	716	721	724	rBV	2454412	2491375	83.33%	11.303%
6	6.899	781	784	788	rBV	814201	639459	21.39%	2.901%
7	7.463	875	880	883	rBV	1878476	1701031	56.89%	7.717%
8	8.081	981	985	992	rBV	120239	139670	4.67%	0.634%
9	8.181	998	1002	1006	rBV	996611	882625	29.52%	4.004%
10	9.257	1180	1185	1189	rBV	3103940	2989904	100.00%	13.565%
11	9.751	1264	1269	1276	rBV5	36224	58448	1.95%	0.265%
12	9.940	1298	1301	1305	rVB	1111280	958322	32.05%	4.348%
13	10.734	1432	1436	1439	rBV	2438580	2028226	67.84%	9.202%
14	11.075	1490	1494	1500	rBV7	20312	40916	1.37%	0.186%
15	11.375	1539	1545	1551	rBV2	60991	97307	3.25%	0.441%
16	11.434	1551	1555	1558	rVB	1225538	960579	32.13%	4.358%
17	11.810	1616	1619	1627	rVB	55145	55602	1.86%	0.252%
18	11.945	1638	1642	1647	rBV	154586	152218	5.09%	0.691%
19	12.098	1665	1668	1673	rBV2	75402	87972	2.94%	0.399%
20	12.139	1673	1675	1683	rVB6	42745	74856	2.50%	0.340%
21	12.804	1782	1788	1789	rBV	88887	140831	4.71%	0.639%
22	13.022	1820	1825	1828	rBV	3424787	2943793	98.46%	13.356%
23	13.633	1923	1929	1938	rVB2	193722	340753	11.40%	1.546%
24	13.939	1973	1981	1988	rBV5	85784	200174	6.69%	0.908%
25	14.033	1993	1997	2001	rVV6	23581	43190	1.44%	0.196%
26	14.080	2001	2005	2008	rVB	706253	640842	21.43%	2.907%
27	14.257	2030	2035	2043	rVB	252531	371526	12.43%	1.686%
28	14.786	2119	2125	2131	rBV	206853	355792	11.90%	1.614%
29	14.845	2131	2135	2140	rBV6	55068	91303	3.05%	0.414%
30	14.922	2146	2148	2155	rVB	40517	46289	1.55%	0.210%
31	15.363	2218	2223	2232	rVB	152670	248972	8.33%	1.130%
32	15.575	2254	2259	2268	rBV	399002	513545	17.18%	2.330%
33	16.033	2331	2337	2344	rVB3	77952	157340	5.26%	0.714%

Sum of corrected areas: 22041751

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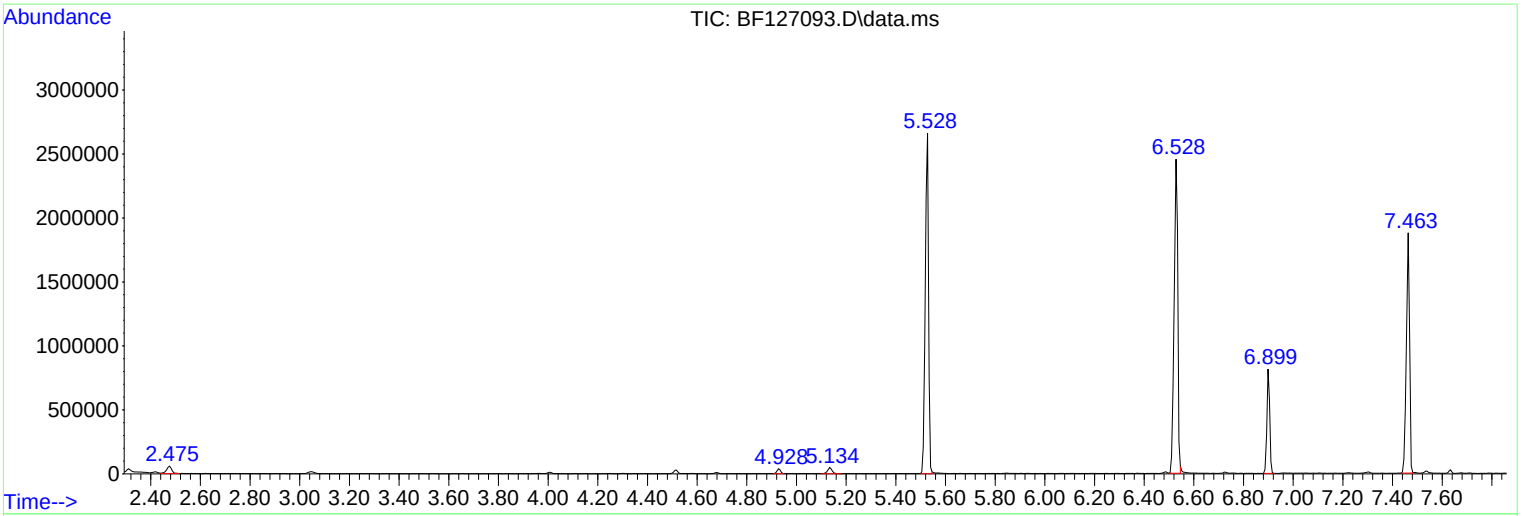
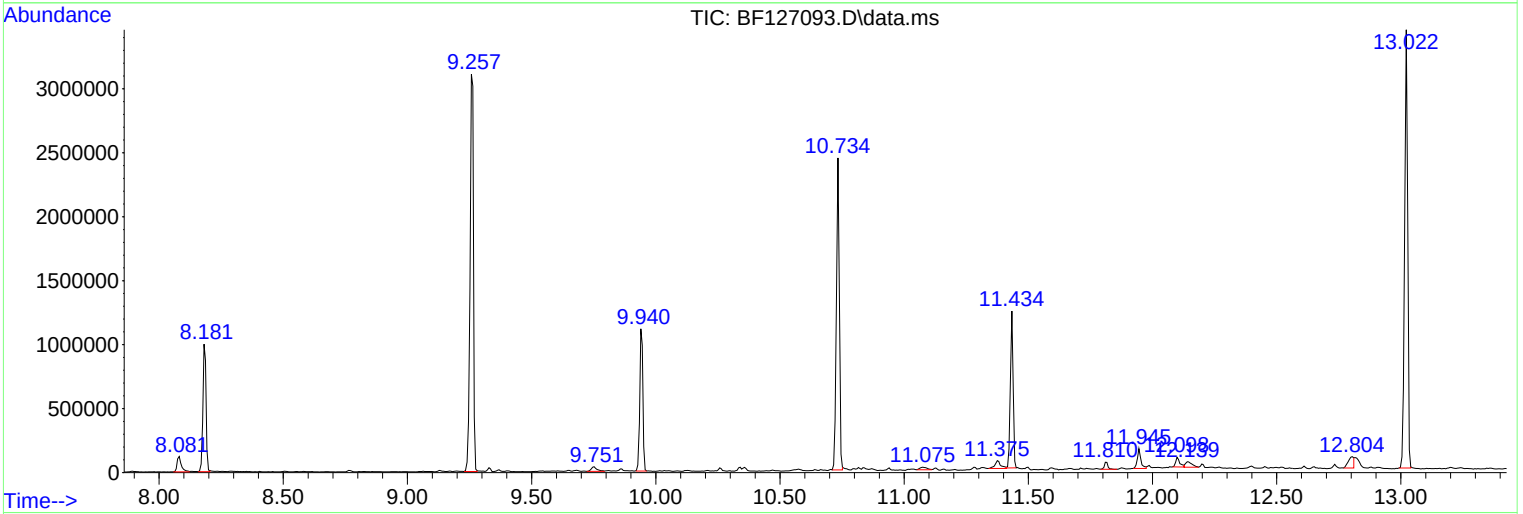
Sample : N1664-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

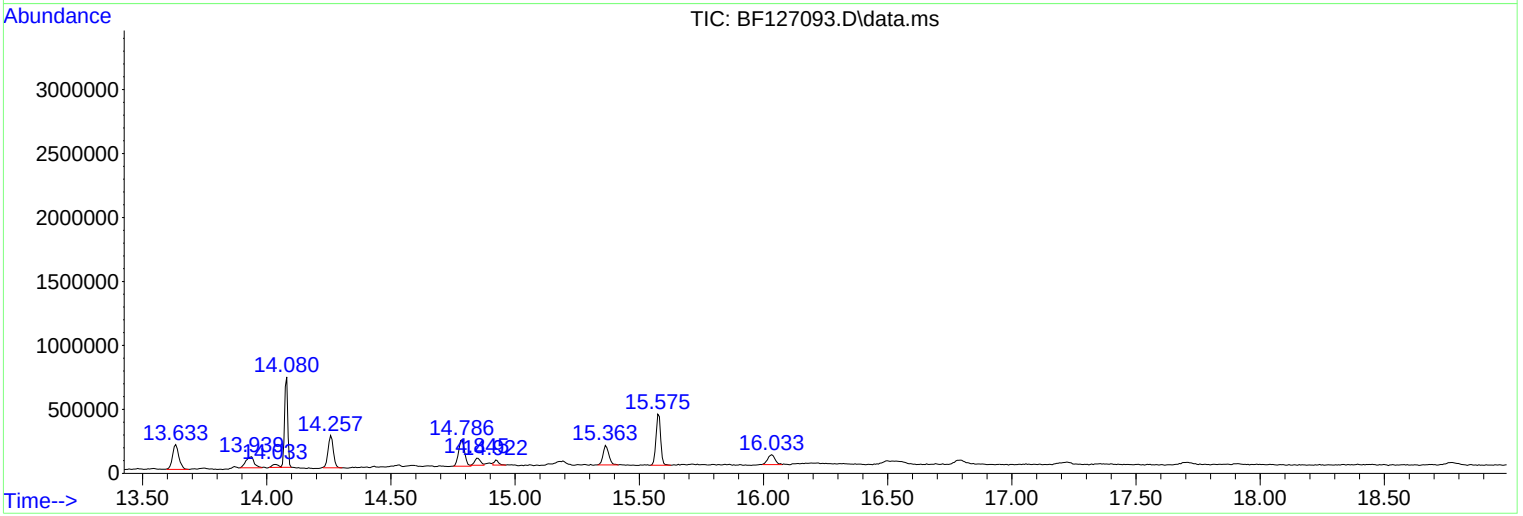
Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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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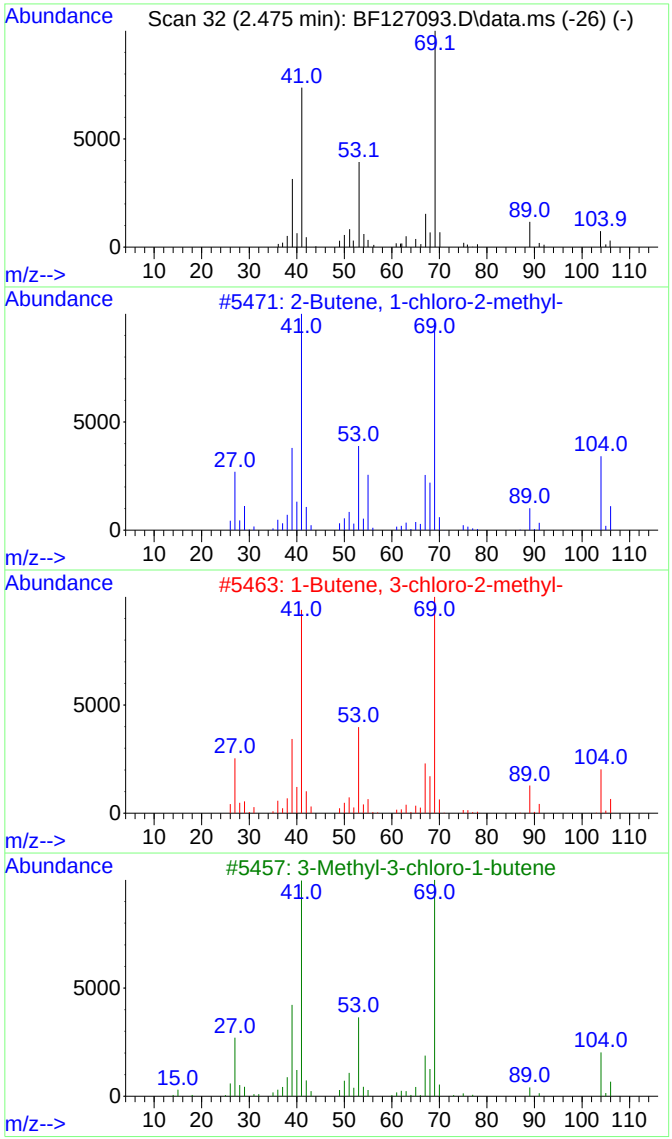
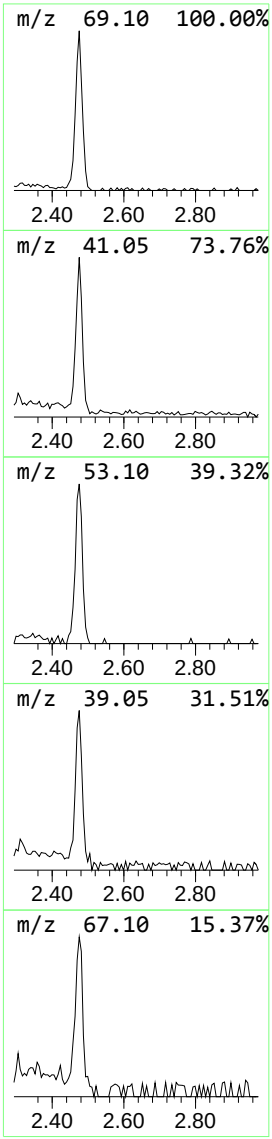
Peak Number 1 2-Butene, 1-chloro-2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.475	2.55 ng	81568	1,4-Dichlorobenzene-d4	6.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 1-chloro-2-methyl-	104	C5H9Cl	013417-43-1	83
2	1-Butene, 3-chloro-2-methyl-	104	C5H9Cl	005166-35-8	83
3	3-Methyl-3-chloro-1-butene	104	C5H9Cl	002190-48-9	74
4	2-Butene, 2-chloro-3-methyl-	104	C5H9Cl	017773-65-8	64
5	1-Butene, 2-chloro-3-methyl-	104	C5H9Cl	017773-64-7	56





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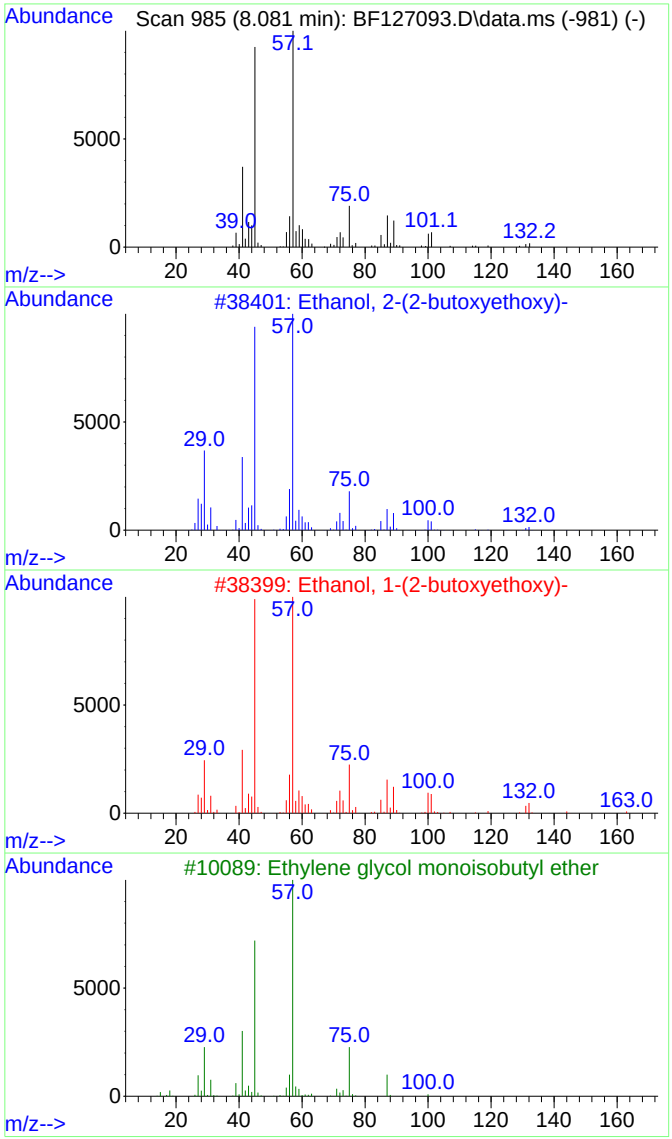
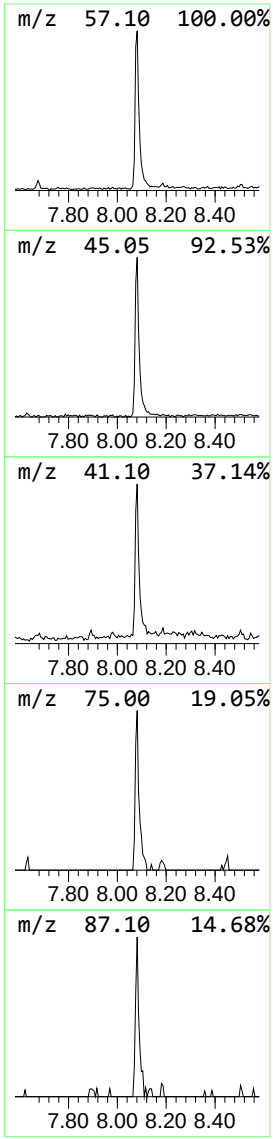
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	3.16 ng	139670	Naphthalene-d8	8.181

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	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	53





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Sample : N1664-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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TIC Library : C:\Database\NIST20.L
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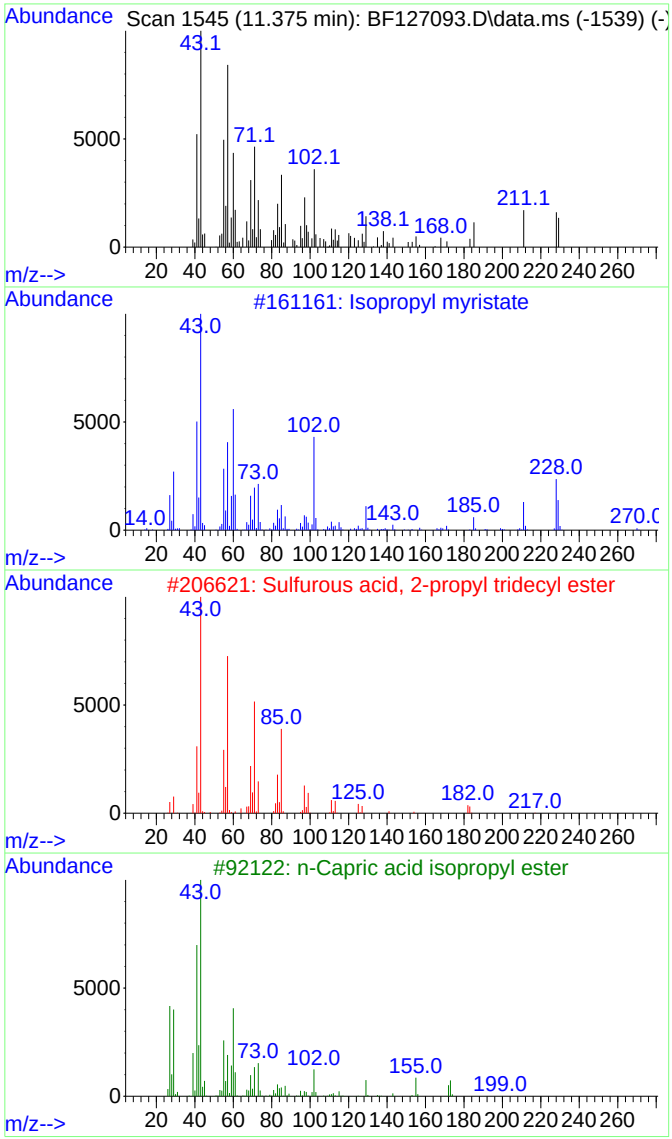
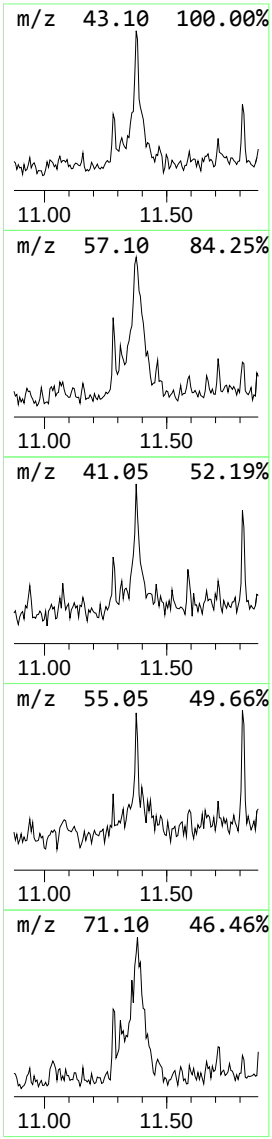
Peak Number 3 Isopropyl myristate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.375	2.03 ng	97307	Phenanthrene-d10	11.434

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl myristate	270	C17H34O2	000110-27-0	52
2	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	30
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	27
4	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	25
5	Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	25





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Instrument :
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ClientSampleId :
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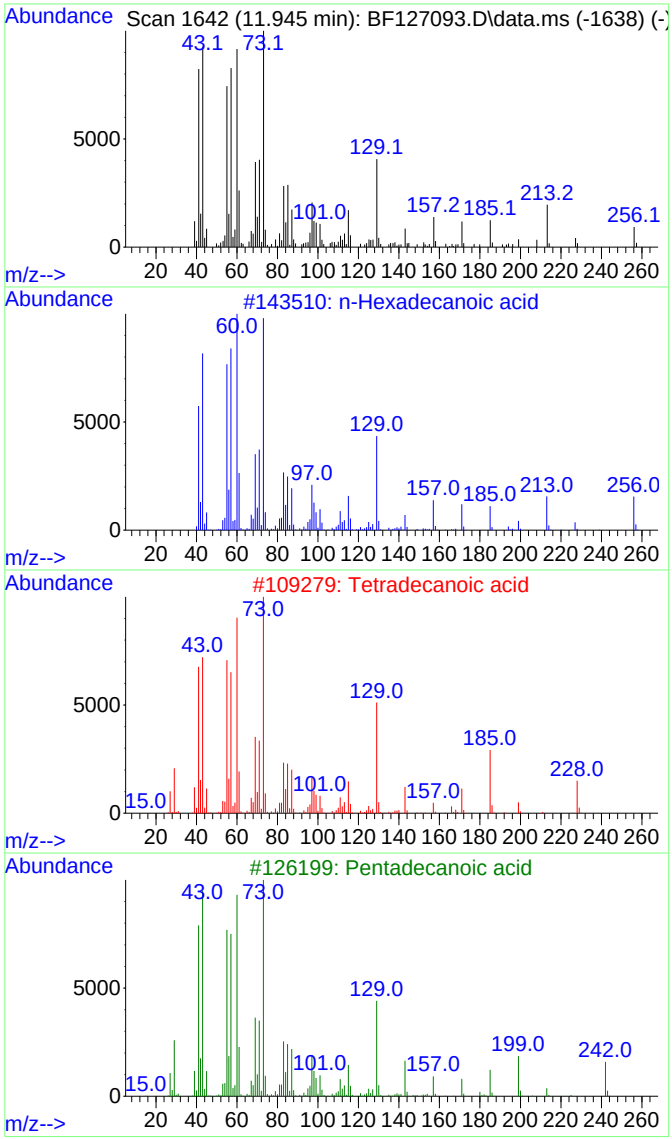
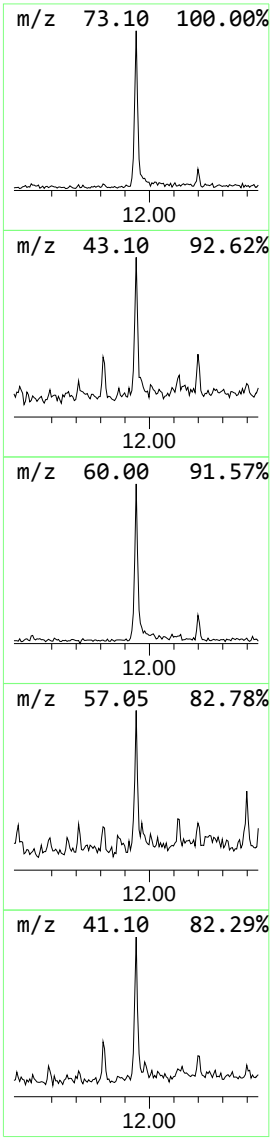
Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	3.17 ng	152218	Phenanthrene-d10	11.434

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





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Instrument :
BNA_F
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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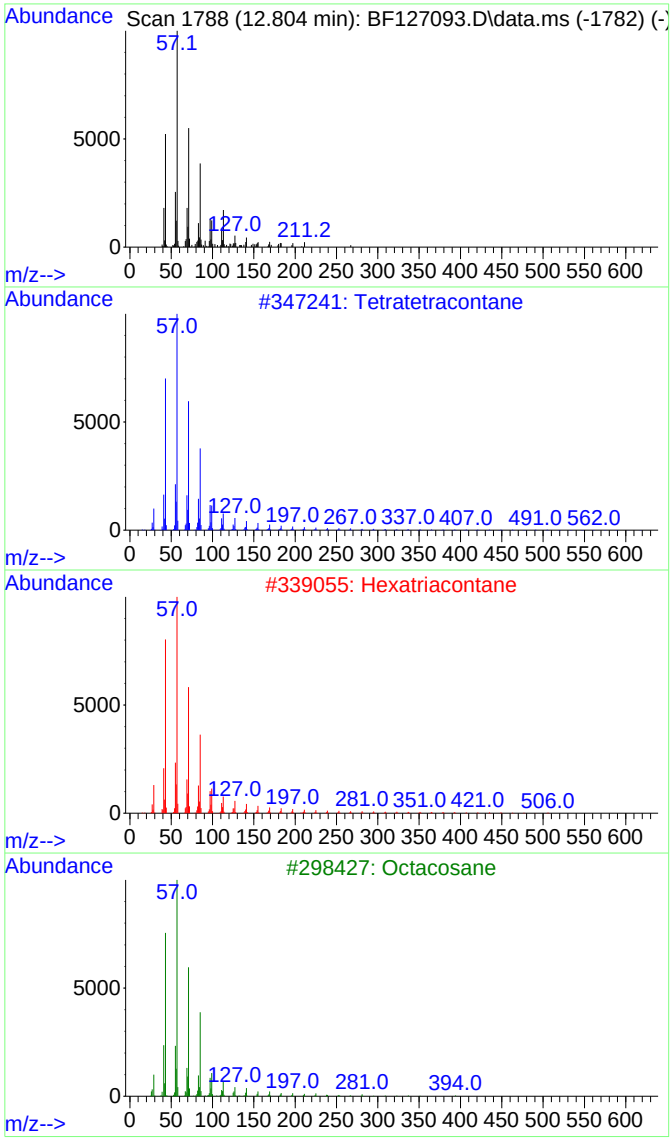
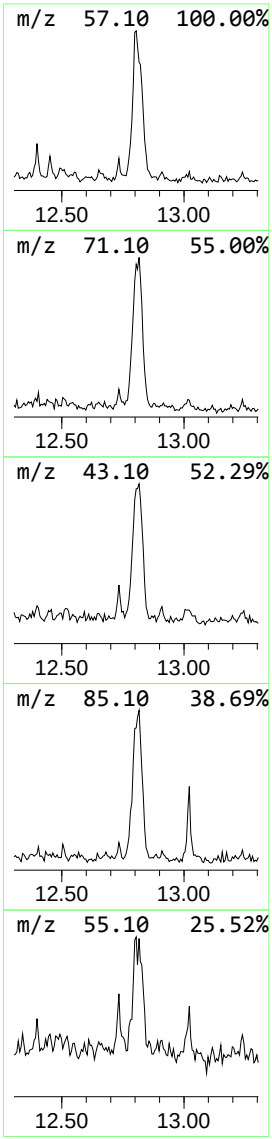
Peak Number 5 Tetratetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.804	4.40 ng	140831	Chrysene-d12	14.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Hexatriacontane	507	C36H74	000630-06-8	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86





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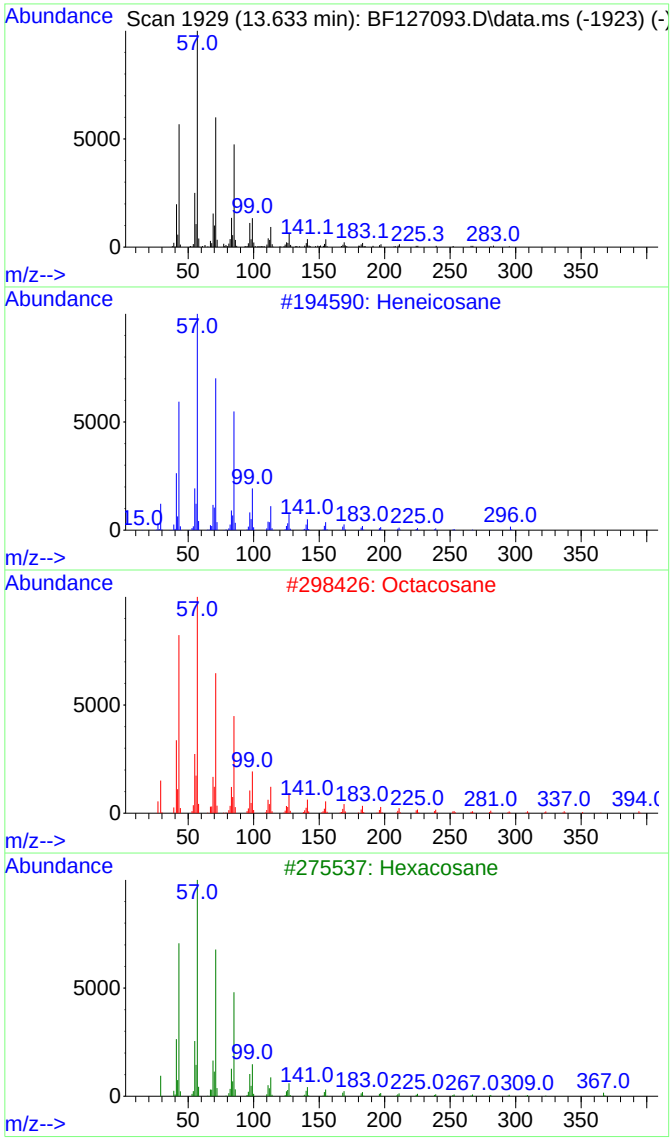
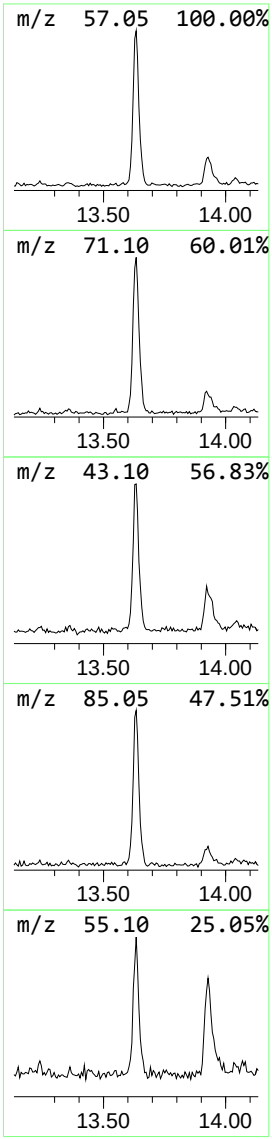
Peak Number 6 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.634	10.63 ng	340753	Chrysene-d12	14.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





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Instrument :
BNA_F
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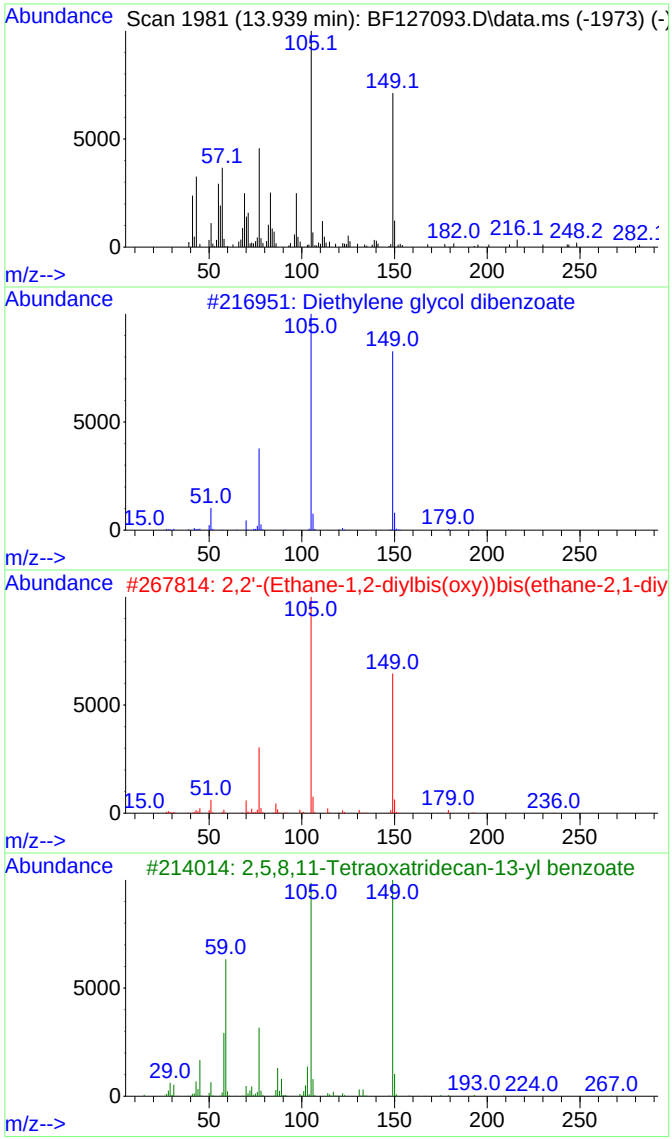
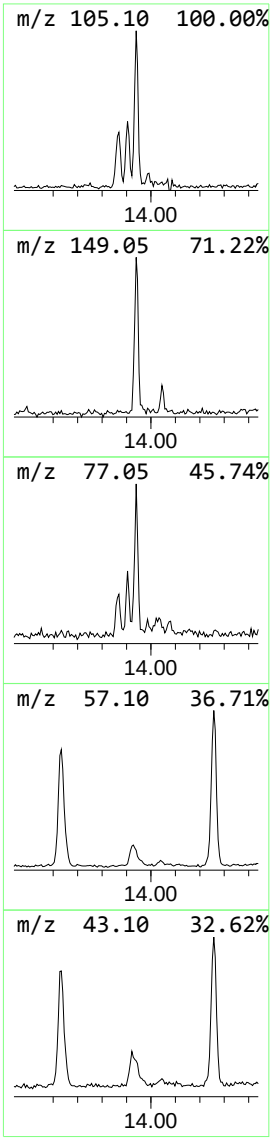
Peak Number 7 unknown13.939 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	6.25 ng	200174	Chrysene-d12	14.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	43
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	35
3	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	27
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	18
5	Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	14





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TIC Library : C:\Database\NIST20.L
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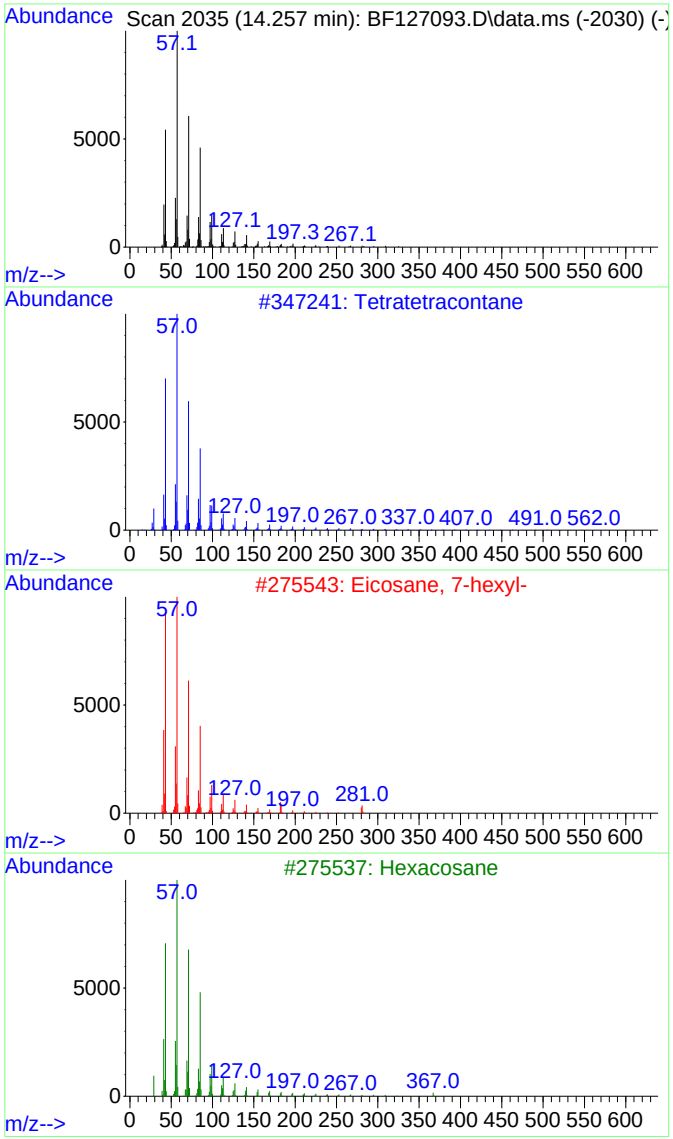
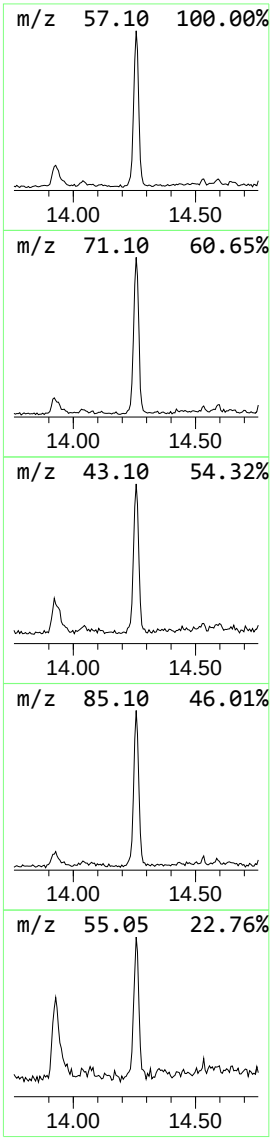
Peak Number 8 Eicosane, 7-hexyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	11.59 ng	371526	Chrysene-d12	14.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5	Octacosane	394	C28H58	000630-02-4	91





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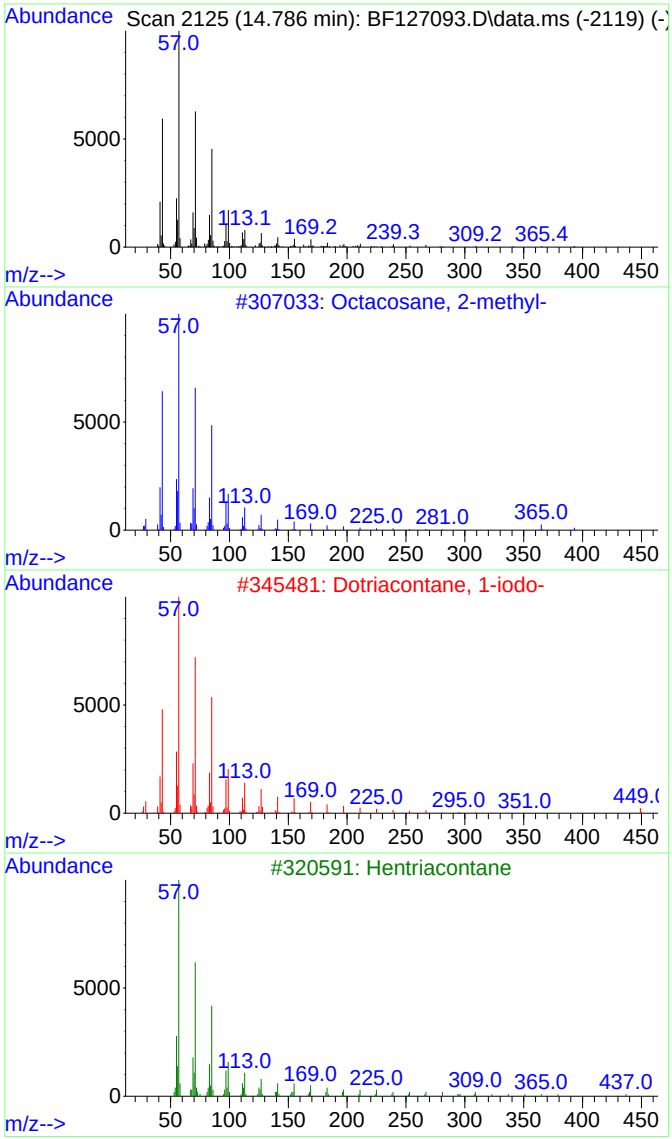
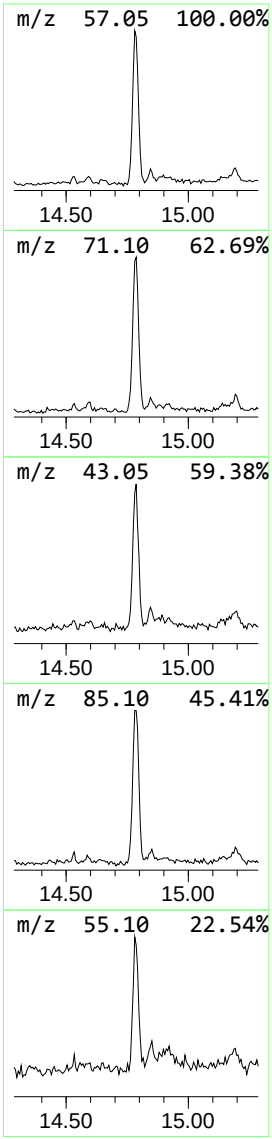
Peak Number 9 Octacosane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	11.10 ng	355792	Chrysene-d12	14.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	4-Methylheneicosane	310	C22H46	025117-29-7	91





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Data File : BF127093.D
Acq On : 28 Feb 2022 12:02
Operator : CG\JU
Sample : N1664-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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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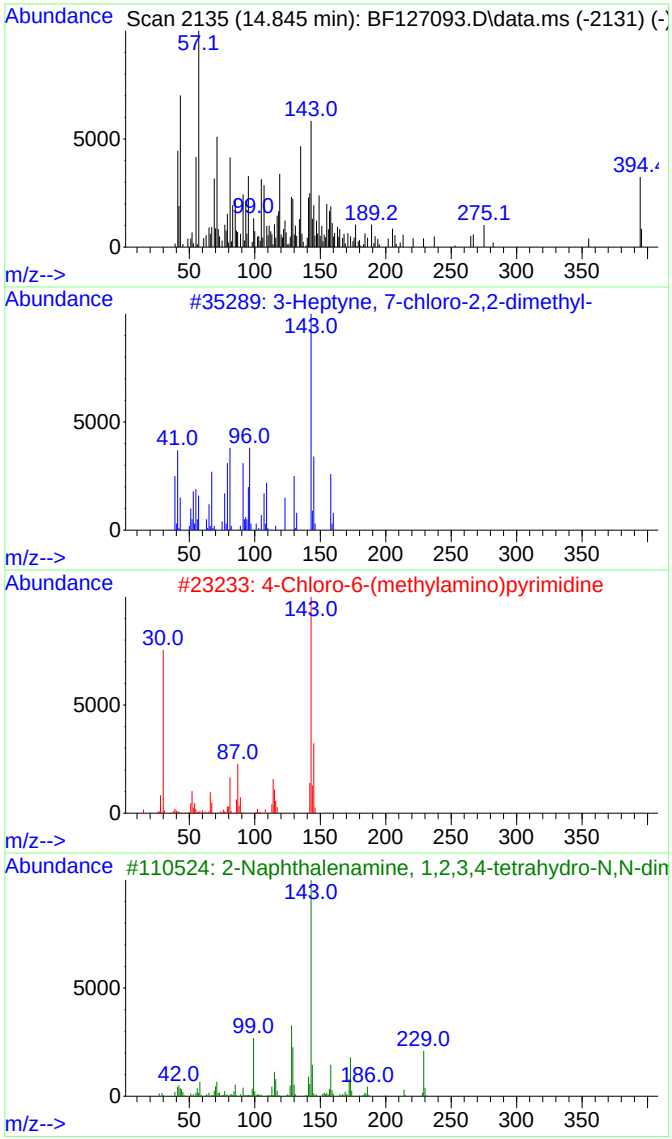
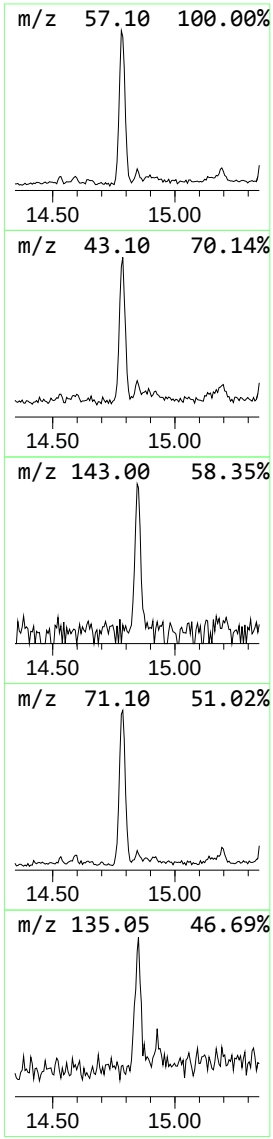
Peak Number 10 unknown14.845 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	3.56 ng	91303	Perylene-d12	15.575

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptyne, 7-chloro-2,2-dimethyl-	158	C9H15Cl	055402-10-3	15
2	4-Chloro-6-(methylamino)pyrimidine	143	C5H6ClN3	065766-32-7	11
3	2-Naphthalenamine, 1,2,3,4-tetra...	229	C16H23N	068157-17-5	11
4	1-Phenyl-1-cyclopropanecarbonitrile	143	C10H9N	000935-44-4	11
5	Isoquinoline, 7-methyl-	143	C10H9N	054004-38-5	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127093.D
Acq On : 28 Feb 2022 12:02
Operator : CG\JU
Sample : N1664-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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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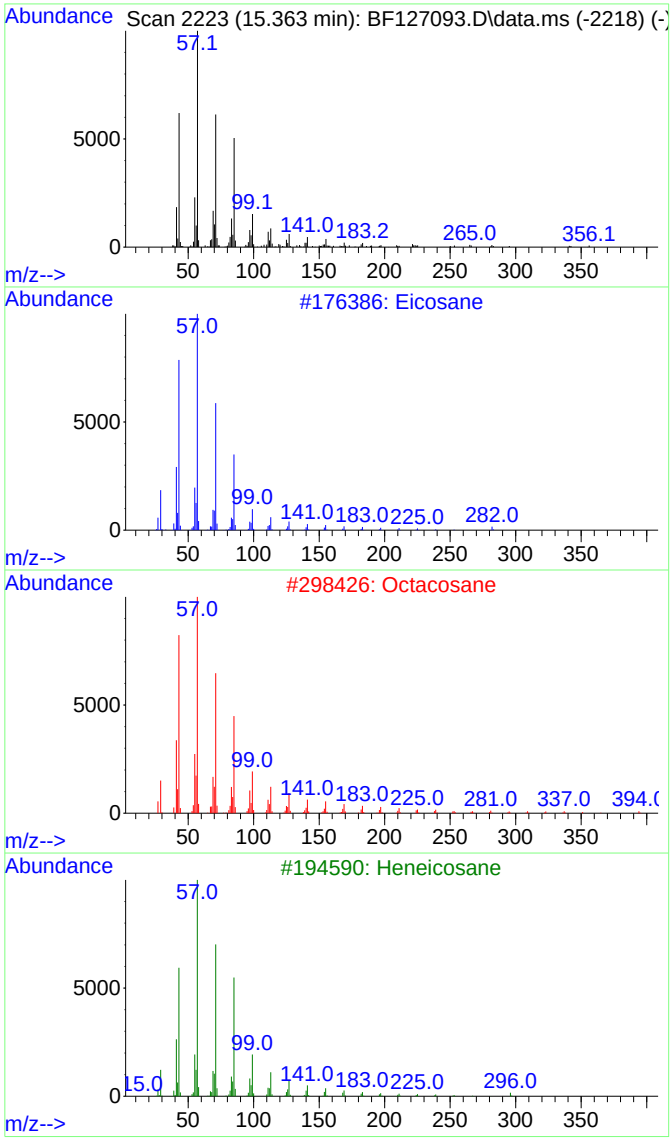
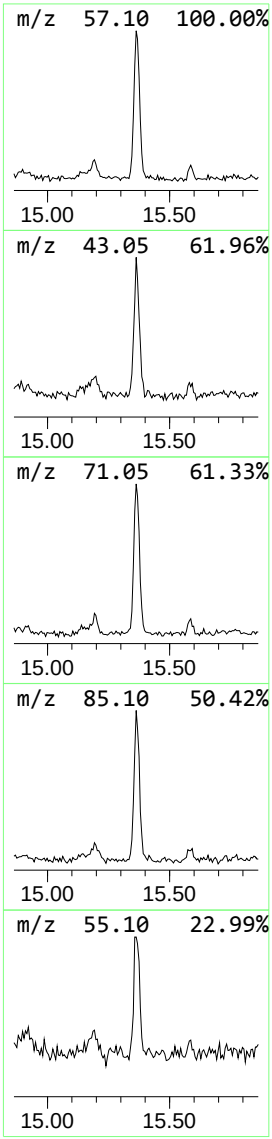
Peak Number 11 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.363	9.70 ng	248972	Perylene-d12	15.575

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127093.D
Acq On : 28 Feb 2022 12:02
Operator : CG\JU
Sample : N1664-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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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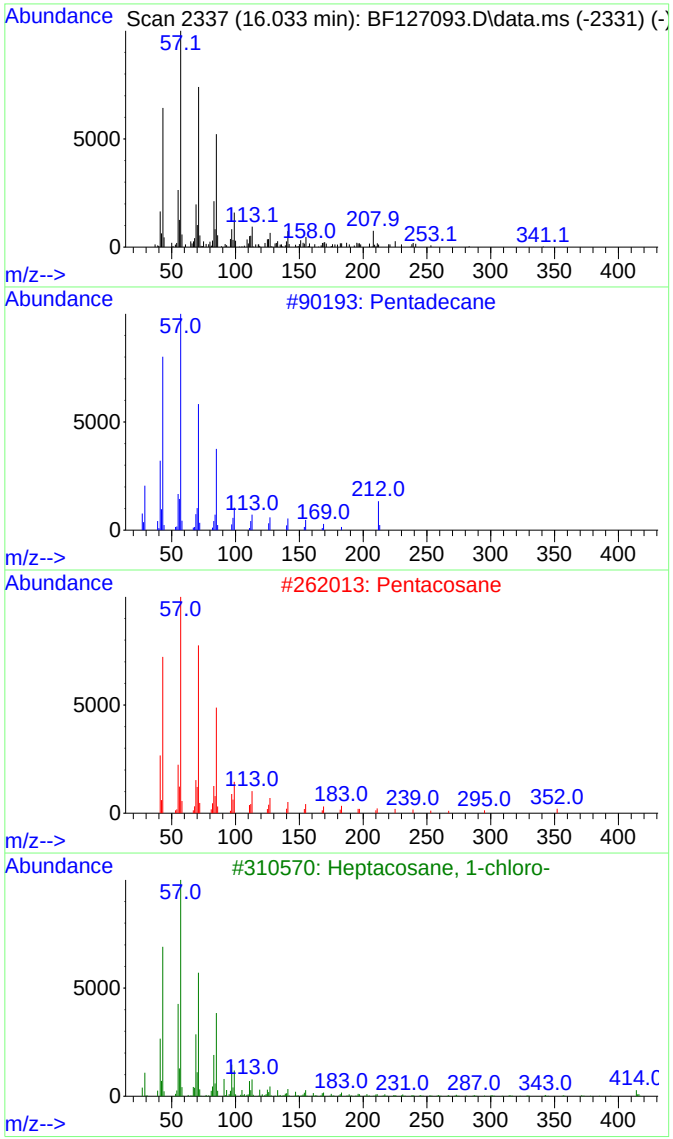
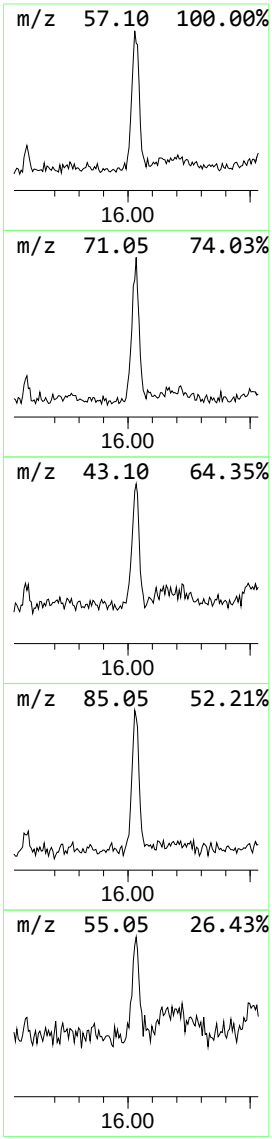
Peak Number 12 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.033	6.13 ng	157340	Perylene-d12	15.575

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Pentacosane	352	C25H52	000629-99-2	87
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86
4	Tetracosane	338	C24H50	000646-31-1	83
5	Hexacosane	366	C26H54	000630-01-3	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127093.D
Acq On : 28 Feb 2022 12:02
Operator : CG\JU
Sample : N1664-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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-Butene, 1-chl...	2.475	2.5	ng	81568	1	6.899	639459	20.0
Ethanol, 2-(2-b...	8.081	3.2	ng	139670	2	8.181	882625	20.0
Isopropyl myris...	11.375	2.0	ng	97307	4	11.434	960579	20.0
n-Hexadecanoic ...	11.945	3.2	ng	152218	4	11.434	960579	20.0
Tetratetracontane	12.804	4.4	ng	140831	5	14.081	640842	20.0
Heneicosane	13.634	10.6	ng	340753	5	14.081	640842	20.0
unknown13.939	13.939	6.3	ng	200174	5	14.081	640842	20.0
Eicosane, 7-hexyl-	14.257	11.6	ng	371526	5	14.081	640842	20.0
Octacosane, 2-m...	14.786	11.1	ng	355792	5	14.081	640842	20.0
unknown14.845	14.845	3.6	ng	91303	6	15.575	513545	20.0
Eicosane	15.363	9.7	ng	248972	6	15.575	513545	20.0
Pentadecane	16.033	6.1	ng	157340	6	15.575	513545	20.0