LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080323\
Data File : BF134611.D
Acq On : 03 Aug 2023 15:09
Operator : CG\JU
Sample : 03686-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-23-0-2-20230721

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134612.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	563	568	571	rBV	3451275	3304796	100.00%	9.381%
2	6.428	733	738	741	rBV	2997819	3196445	96.72%	9.073%
3	6.798	797	801	805	rBV	2168948	1764136	53.38%	5.008%
4	6.957	825	828	833	rVB3	30366	38866	1.18%	0.110%
5	7.357	891	896	899	rBV	2132491	1905194	57.65%	5.408%
6	8.075	1014	1018	1022	rBV	2368367	2061840	62.39%	5.853%
7	9.151	1197	1201	1205	rBV	3564777	3252860	98.43%	9.233%
8	9.551	1265	1269	1272	rBV	639467	500613	15.15%	1.421%
9	9.833	1313	1317	1320	rBV	2385989	1943297	58.80%	5.516%
10	10.622	1447	1451	1454	rBV	2130263	1825767	55.25%	5.183%
11	10.745	1469	1472	1481	rVB6	26061	37524	1.14%	0.107%
12	11.192	1545	1548	1551	rBV	57015	58657	1.77%	0.167%
13	11.322	1566	1570	1572	rBV	2337558	1952062	59.07%	5.541%
14	11.345	1572	1574	1577	rVB	255844	184225	5.57%	0.523%
15	11.392	1578	1582	1585	rVB2	59168	65780	1.99%	0.187%
16	11.551	1604	1609	1612	rBV2	54792	69325	2.10%	0.197%
17	11.622	1619	1621	1623	rBV	58025	44510	1.35%	0.126%
18	11.822	1652	1655	1657	rBV	69242	56388	1.71%	0.160%
19	11.857	1657	1661	1665	rBV2	335584	311378	9.42%	0.884%
20	12.533	1773	1776	1779	rBV	298082	273166	8.27%	0.775%
21	12.633	1790	1793	1794	rBV2	79972	80584	2.44%	0.229%
22	12.733	1807	1810	1811	rBV	136043	111414	3.37%	0.316%
23	12.763	1813	1815	1819	rVB	282232	251930	7.62%	0.715%
24	12.916	1837	1841	1844	rBV	3666131	3036478	91.88%	8.619%
25	13.821	1992	1995	2002	rBV3	622985	744745	22.54%	2.114%
26	13.968	2016	2020	2023	rVB	1415273	1420168	42.97%	4.031%
27	14.463	2100	2104	2110	rVB	719037	802736	24.29%	2.279%
28	14.915	2177	2181	2185	rBV	1044768	1191140	36.04%	3.381%
29	15.133	2212	2218	2226	rVB3	1595449	2615091	79.13%	7.423%
30	15.439	2267	2270	2277	rVB	796906	934993	28.29%	2.654%
31	15.710	2312	2316	2322	rVB4	425745	628330	19.01%	1.784%
32	15.951	2353	2357	2361	rBV	402138	564744	17.09%	1.603%

Sum of corrected areas: 35229182

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080323\
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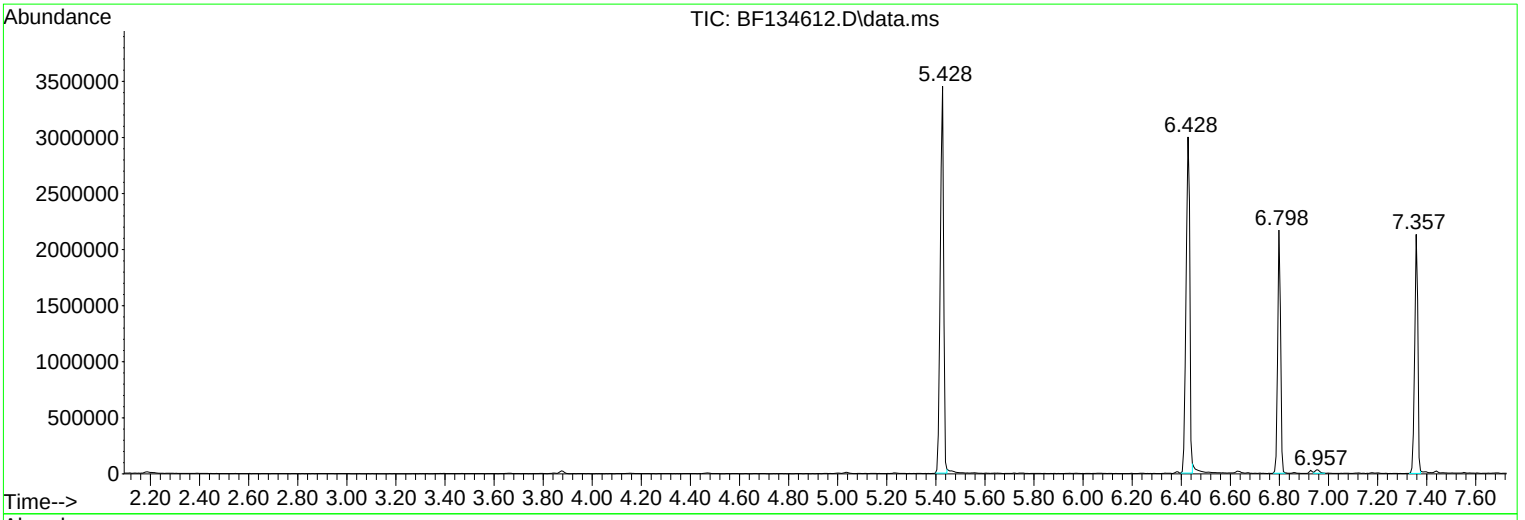
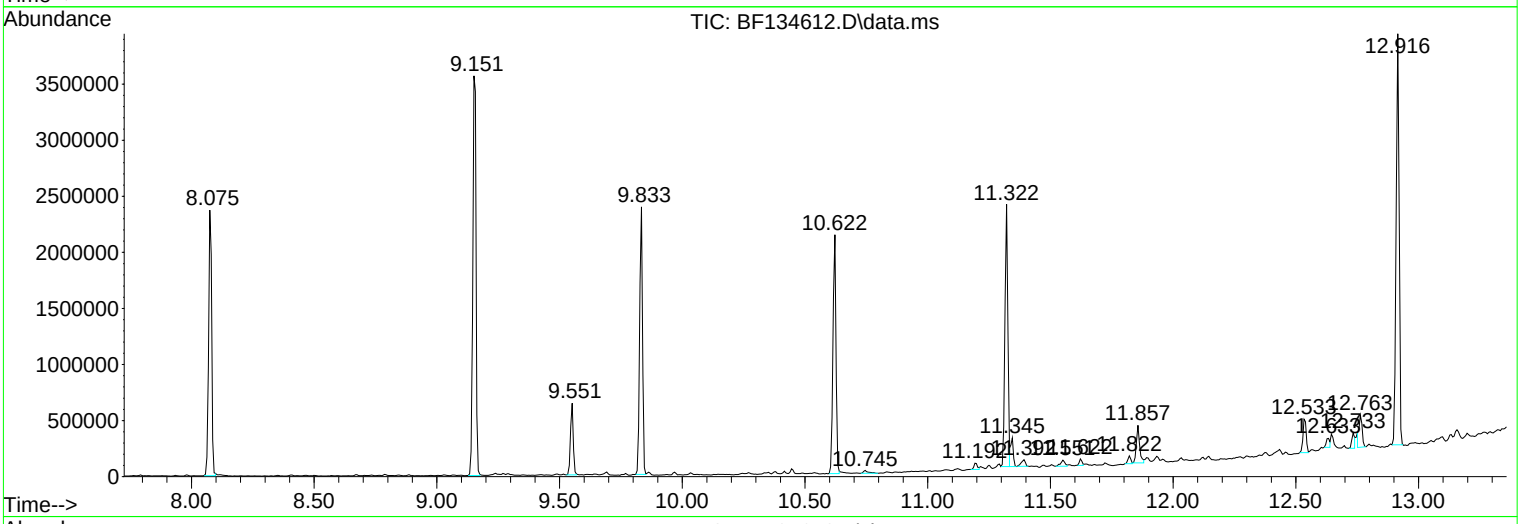
Misc :
ALS Vial : 14 Sample Multiplier: 1

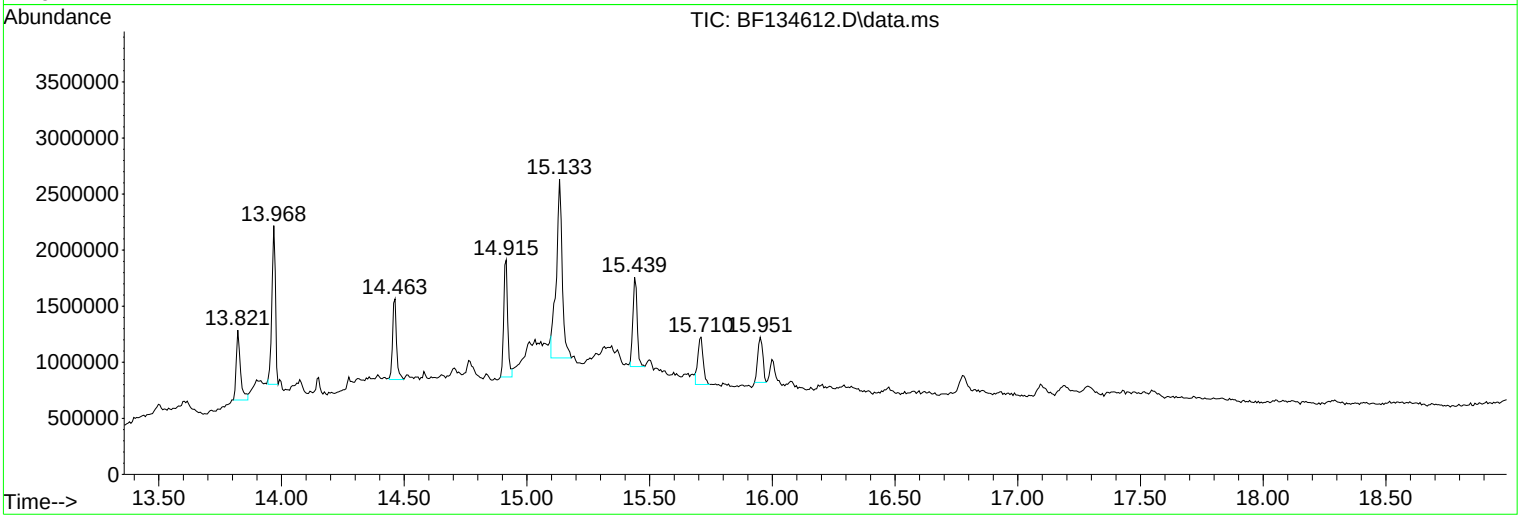
Instrument :
BNA_F
ClientSampleId :
SB-23-0-2-20230721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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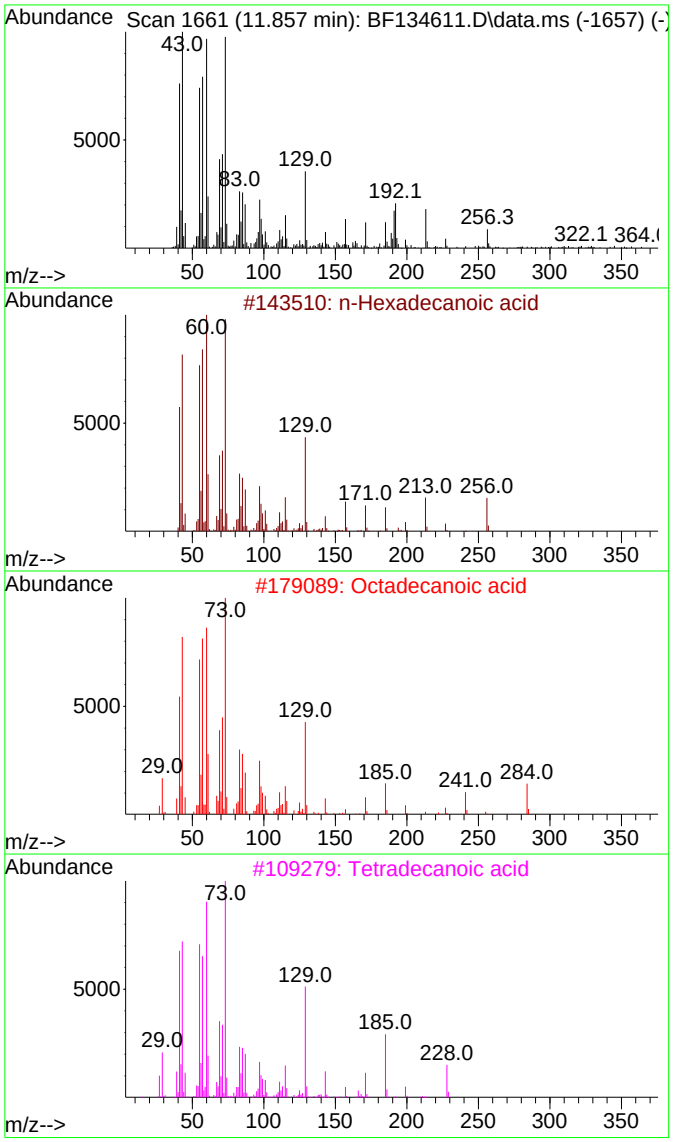
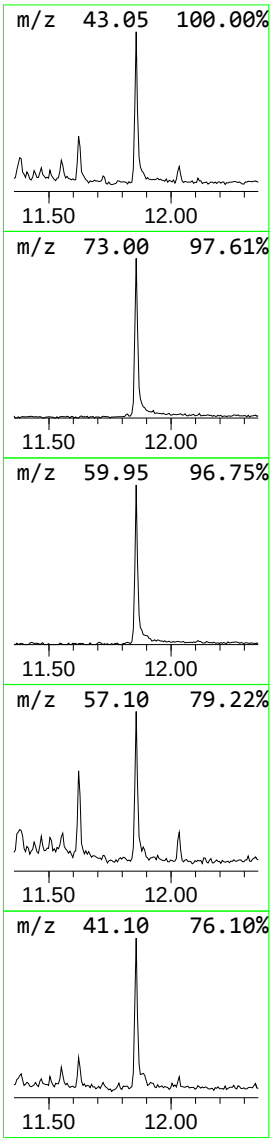
Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	3.19 ng	311378	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





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SB-23-0-2-20230721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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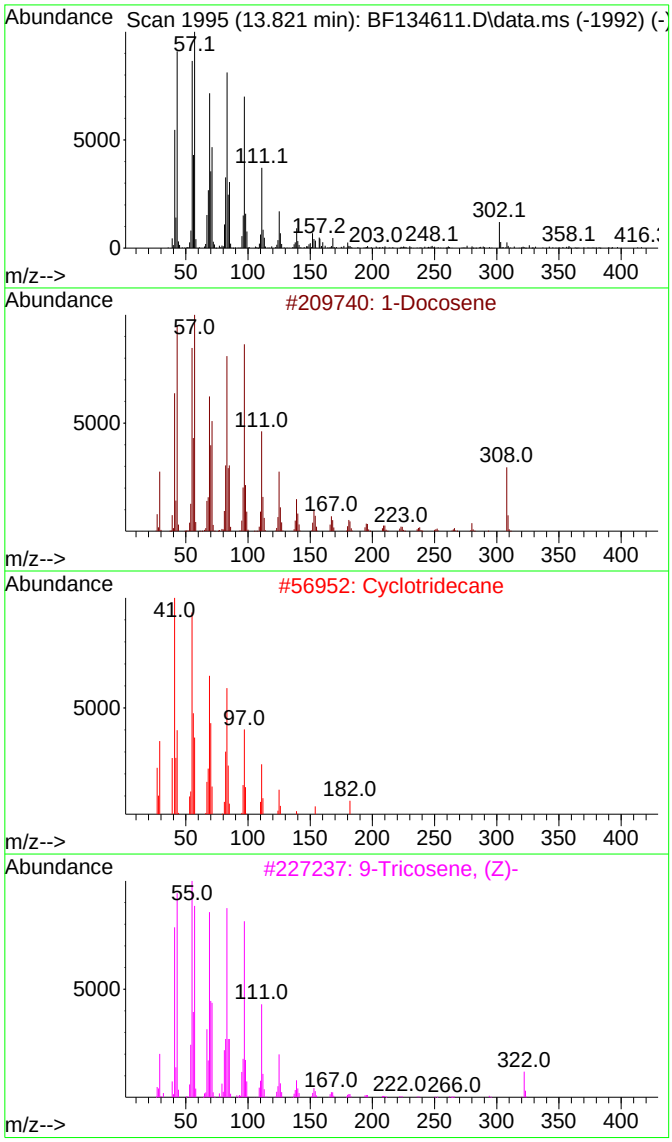
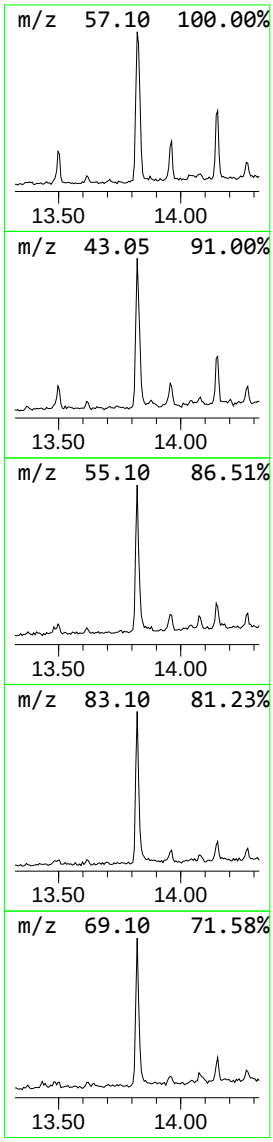
Peak Number 2 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	10.49 ng	744745	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	98
2	Cyclotridecane	182	C13H26	000295-02-3	95
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	94





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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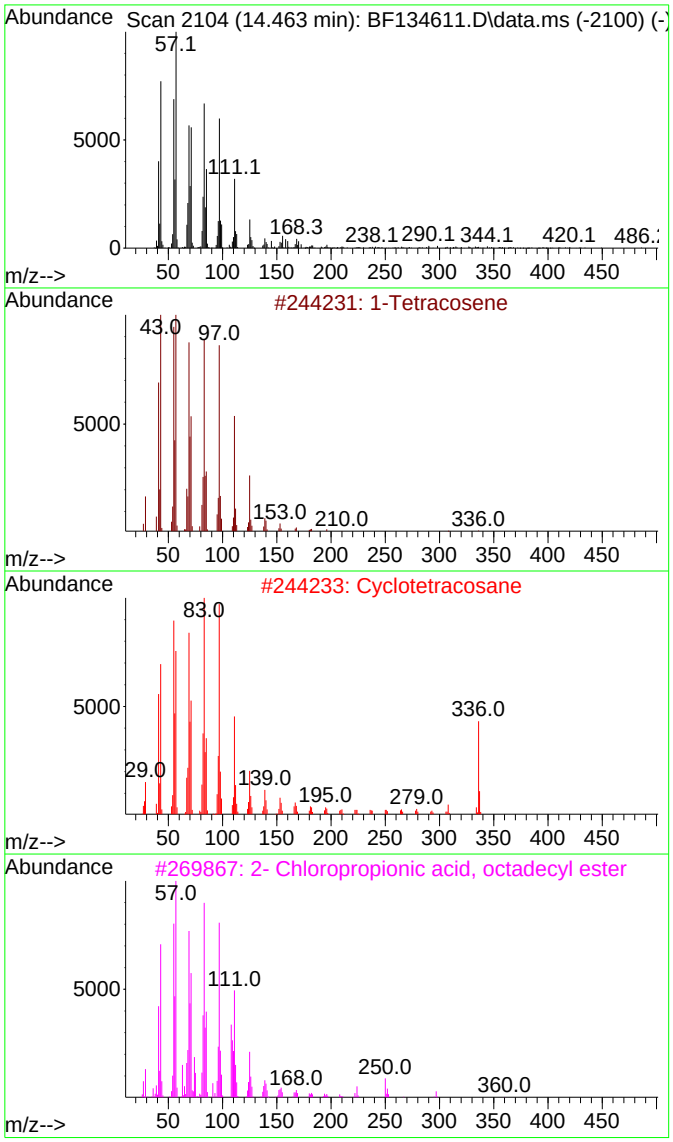
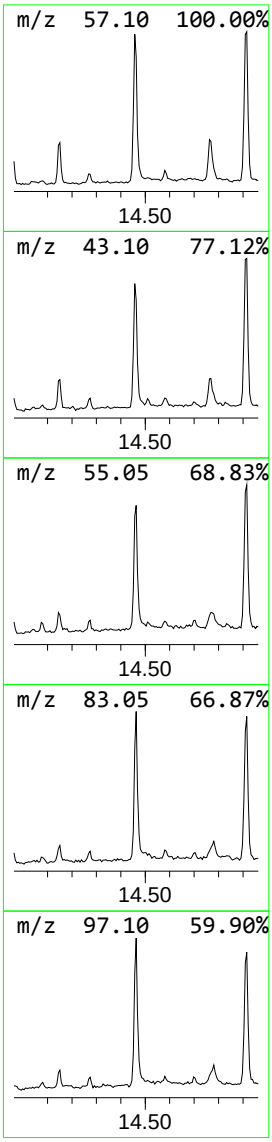
Peak Number 3 1-Tetracosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.463	11.30 ng	802736	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	96
2	Cyclotetracosane	336	C24H48	000297-03-0	95
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4	Cyclopentadecane	210	C15H30	000295-48-7	93
5	13-Methyl-Z-14-nonacosene	420	C30H60	1010131-19-0	93





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Data File : BF134611.D
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Sample : 03686-11
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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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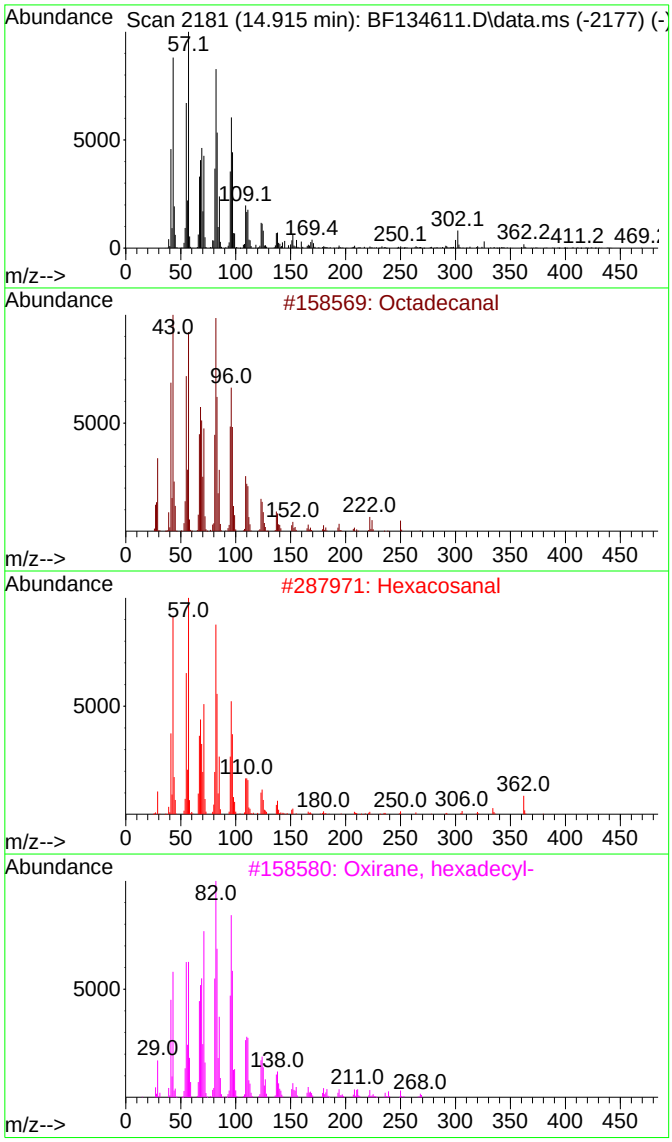
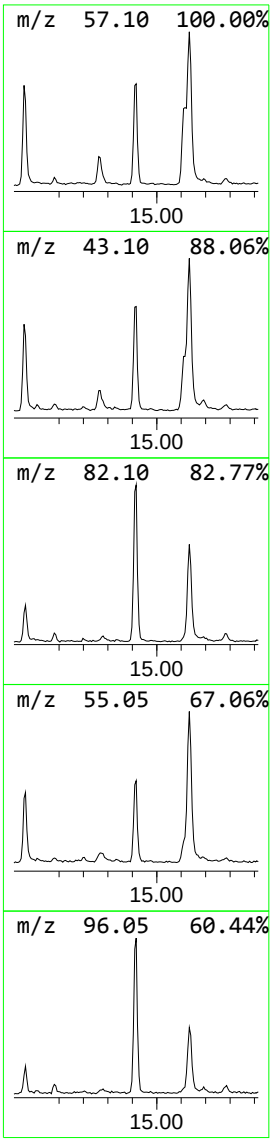
Peak Number 4 Octadecanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	25.48 ng	1191140	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	96
2	Hexacosanal	380	C26H52O	026627-85-0	94
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
4	Eicosanal-	296	C20H40O	002400-66-0	90
5	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080323\
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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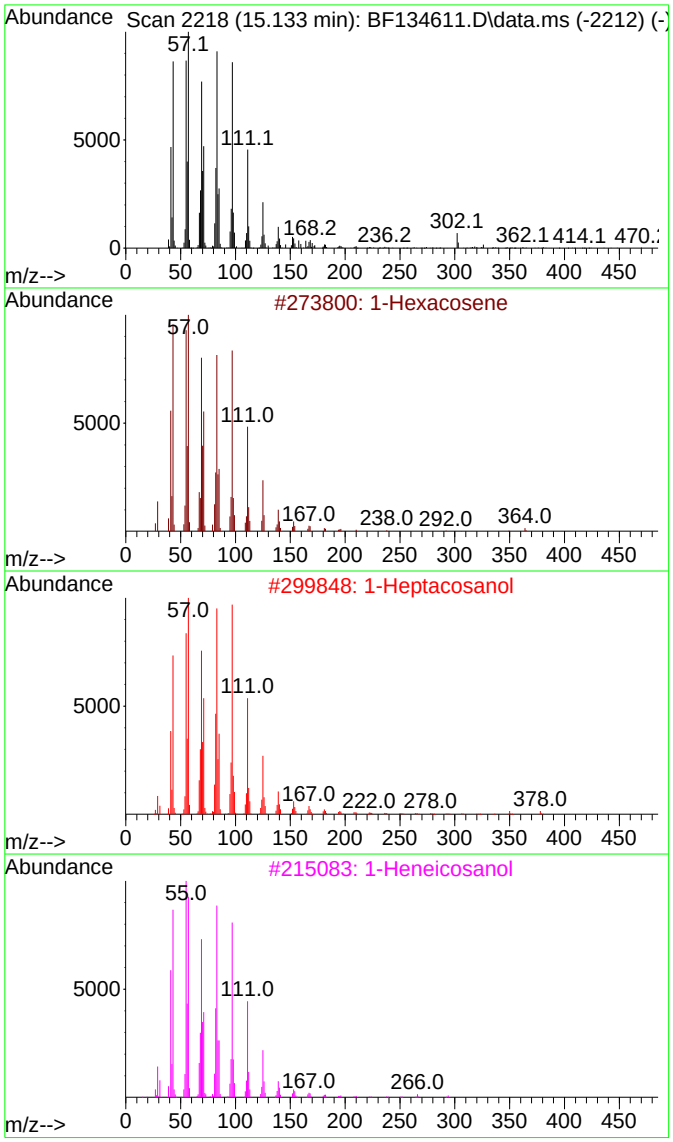
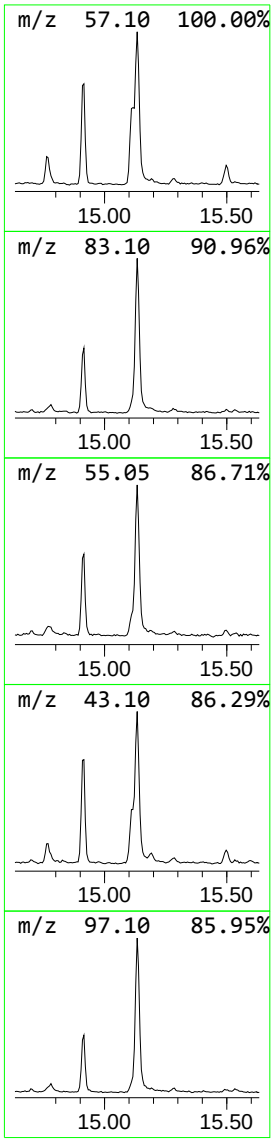
Peak Number 5 1-Hexacosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	55.94 ng	2615090	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Heptacos-1-ene	378	C27H54	015306-27-1	94
5	1-Tetracosene	336	C24H48	010192-32-2	94





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TIC Library : C:\Database\NIST20.L
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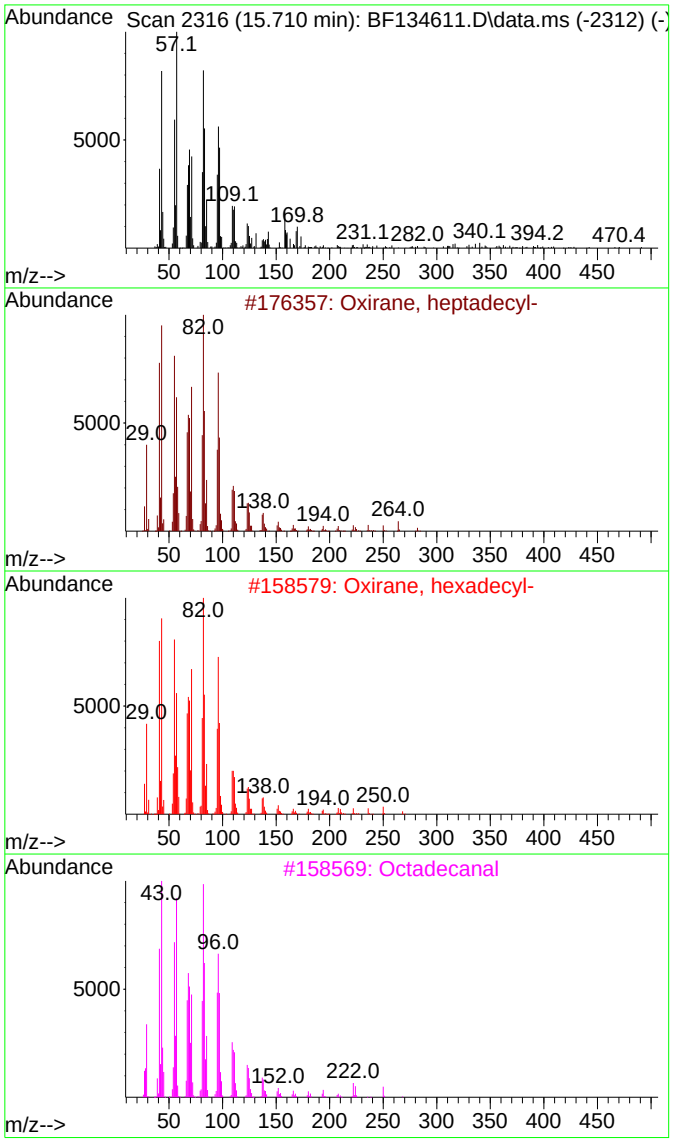
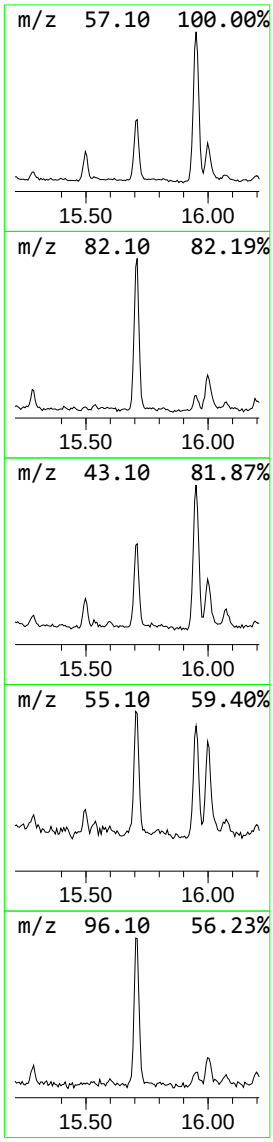
Peak Number 6 Oxirane, heptadecyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.710	13.44 ng	628330	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Octadecanal	268	C18H36O	000638-66-4	91
4	Tetracosanal	352	C24H48O	057866-08-7	87
5	13-Octadecenal	266	C18H34O	056554-90-6	86





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

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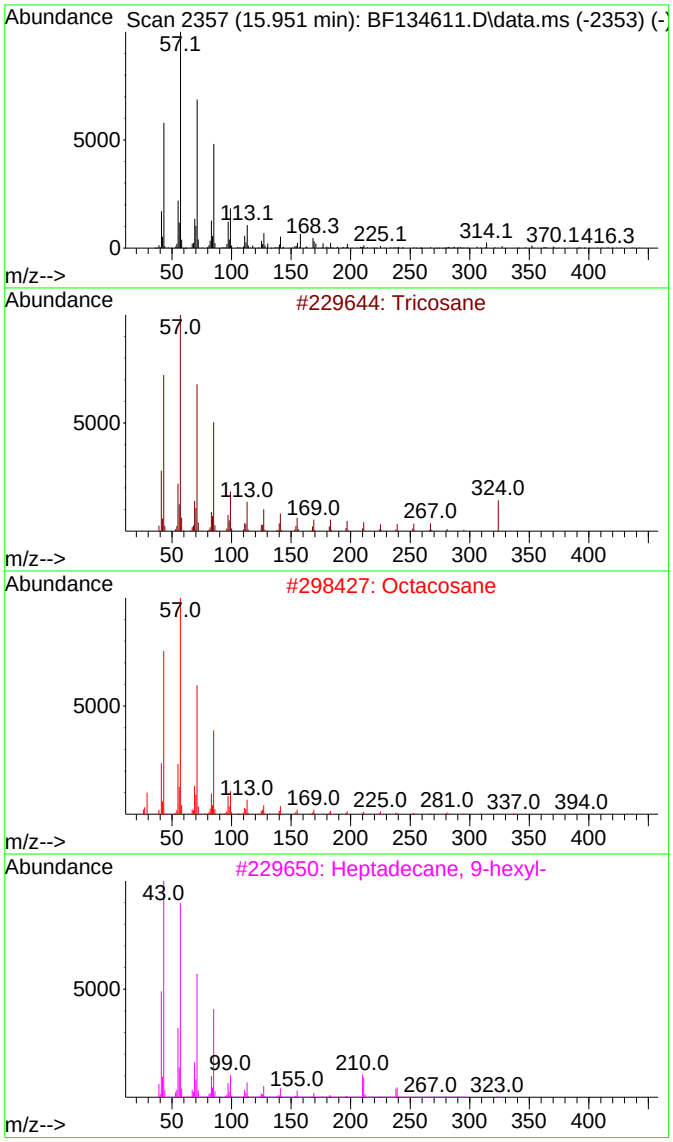
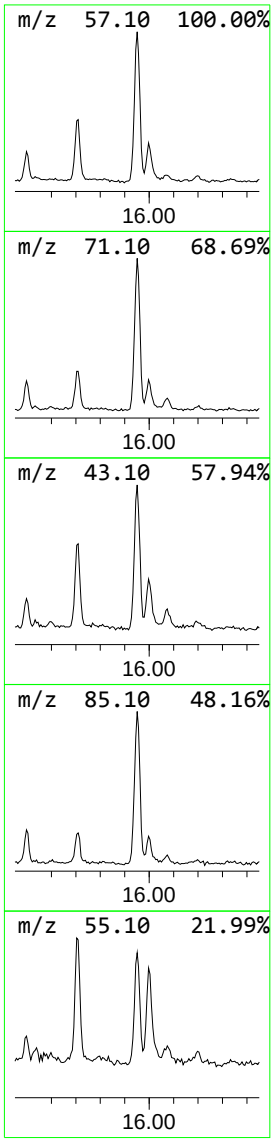
Peak Number 7 Tricosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	12.08 ng	564744	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	94
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Pentacosane	352	C25H52	000629-99-2	89





Tentatively Identified Compound (LSC) summary

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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
n-Hexadecanoic ...	11.857	3.2	ng	311378	4	11.322	1952060	20.0
1-Docosene	13.821	10.5	ng	744745	5	13.969	1420170	20.0
1-Tetracosene	14.463	11.3	ng	802736	5	13.969	1420170	20.0
Octadecanal	14.916	25.5	ng	1191140	6	15.439	934993	20.0
1-Hexacosene	15.133	55.9	ng	2615090	6	15.439	934993	20.0
Oxirane, heptad...	15.710	13.4	ng	628330	6	15.439	934993	20.0
Tricosane	15.951	12.1	ng	564744	6	15.439	934993	20.0