LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080323\
Data File : BF134618.D
Acq On : 03 Aug 2023 18:53
Operator : CG\JU
Sample : 03686-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-29-0-2-20230721

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: BF134619.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.422	562	567	570	rBV	2928334	2854136	100.00%	10.291%
2	6.428	733	738	741	rBV	2956920	2792470	97.84%	10.069%
3	6.798	796	801	804	rBV	1303987	1034913	36.26%	3.732%
4	7.357	891	896	899	rBV	1927264	1641762	57.52%	5.920%
5	8.075	1014	1018	1021	rBV	1543177	1197685	41.96%	4.318%
6	9.151	1197	1201	1204	rBV	3305694	2761977	96.77%	9.959%
7	9.545	1265	1268	1272	rBV	465453	409454	14.35%	1.476%
8	9.692	1288	1293	1297	rVB	38380	37581	1.32%	0.136%
9	9.828	1313	1316	1320	rBV	1261985	1098230	38.48%	3.960%
10	10.616	1446	1450	1454	rBV	1905380	1606968	56.30%	5.794%
11	10.745	1469	1472	1479	rVB4	30820	41353	1.45%	0.149%
12	11.192	1545	1548	1550	rBV	47043	38041	1.33%	0.137%
13	11.316	1566	1569	1572	rBV	1290779	1165590	40.84%	4.203%
14	11.339	1572	1573	1576	rVV	269932	189085	6.62%	0.682%
15	11.392	1576	1582	1584	rVB2	68831	76974	2.70%	0.278%
16	11.551	1603	1609	1611	rBV3	37340	47058	1.65%	0.170%
17	11.622	1618	1621	1623	rBV2	51643	40201	1.41%	0.145%
18	11.822	1651	1655	1657	rBV	120762	105658	3.70%	0.381%
19	11.857	1657	1661	1665	rVV2	412780	426726	14.95%	1.539%
20	11.892	1665	1667	1670	rVV2	74263	76148	2.67%	0.275%
21	11.933	1670	1674	1676	rVV	74265	87966	3.08%	0.317%
22	11.957	1676	1678	1683	rVB	41977	40380	1.41%	0.146%
23	12.051	1692	1694	1700	rVB6	28392	37322	1.31%	0.135%
24	12.122	1702	1706	1707	rVV	36860	39136	1.37%	0.141%
25	12.139	1707	1709	1713	rVB	56994	53022	1.86%	0.191%
26	12.351	1742	1745	1747	rBV3	33254	35605	1.25%	0.128%
27	12.374	1747	1749	1752	rVV	56139	55320	1.94%	0.199%
28	12.433	1756	1759	1761	rVV3	50243	58551	2.05%	0.211%
29	12.457	1761	1763	1768	rVB4	37021	43122	1.51%	0.155%
30	12.533	1773	1776	1779	rVB	506082	395692	13.86%	1.427%
31	12.604	1785	1788	1790	rBV	80823	68472	2.40%	0.247%
32	12.627	1790	1792	1797	rVV2	221252	221149	7.75%	0.797%
33	12.733	1806	1810	1811	rBV	297052	273888	9.60%	0.988%
34	12.763	1811	1815	1818	rVB	458460	575197	20.15%	2.074%
35	12.916	1837	1841	1844	rVB	2707455	2617595	91.71%	9.438%
36	13.092	1869	1871	1874	rVB	53497	44699	1.57%	0.161%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080323\
Data File : BF134618.D
Acq On : 03 Aug 2023 18:53
Operator : CG\JU
Sample : 03686-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-0-2-20230721

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

37	13.127	1875	1877	1879	rBV3	34523	33398	1.17%	0.120%
38	13.157	1879	1882	1885	rVV2	62285	66869	2.34%	0.241%
39	13.198	1886	1889	1891	rVV	50885	46459	1.63%	0.168%
40	13.239	1893	1896	1898	rVV2	65983	58544	2.05%	0.211%
41	13.292	1902	1905	1907	rVB	35840	34823	1.22%	0.126%
42	13.598	1955	1957	1959	rBV	35576	37732	1.32%	0.136%
43	13.821	1991	1995	2000	rBV2	460545	495064	17.35%	1.785%
44	13.963	2014	2019	2022	rBV2	969000	1054646	36.95%	3.803%
45	13.992	2022	2024	2030	rVB	174064	152074	5.33%	0.548%
46	14.145	2048	2050	2053	rBV2	95967	93587	3.28%	0.337%
47	14.457	2100	2103	2108	rBV	269068	302699	10.61%	1.091%
48	14.910	2177	2180	2184	rVB	583893	583047	20.43%	2.102%
49	15.004	2193	2196	2199	rBV	134855	185507	6.50%	0.669%
50	15.110	2210	2214	2215	rBV	273871	285210	9.99%	1.028%
51	15.133	2215	2218	2225	rVB	579838	730040	25.58%	2.632%
52	15.368	2255	2258	2262	rVB	94454	113597	3.98%	0.410%
53	15.433	2265	2269	2273	rBV	465840	529329	18.55%	1.909%
54	15.704	2312	2315	2321	rVB2	170736	228474	8.01%	0.824%
55	15.951	2353	2357	2361	rVV	166259	230247	8.07%	0.830%
56	15.998	2362	2365	2371	rVB2	117927	183819	6.44%	0.663%

Sum of corrected areas: 27734291

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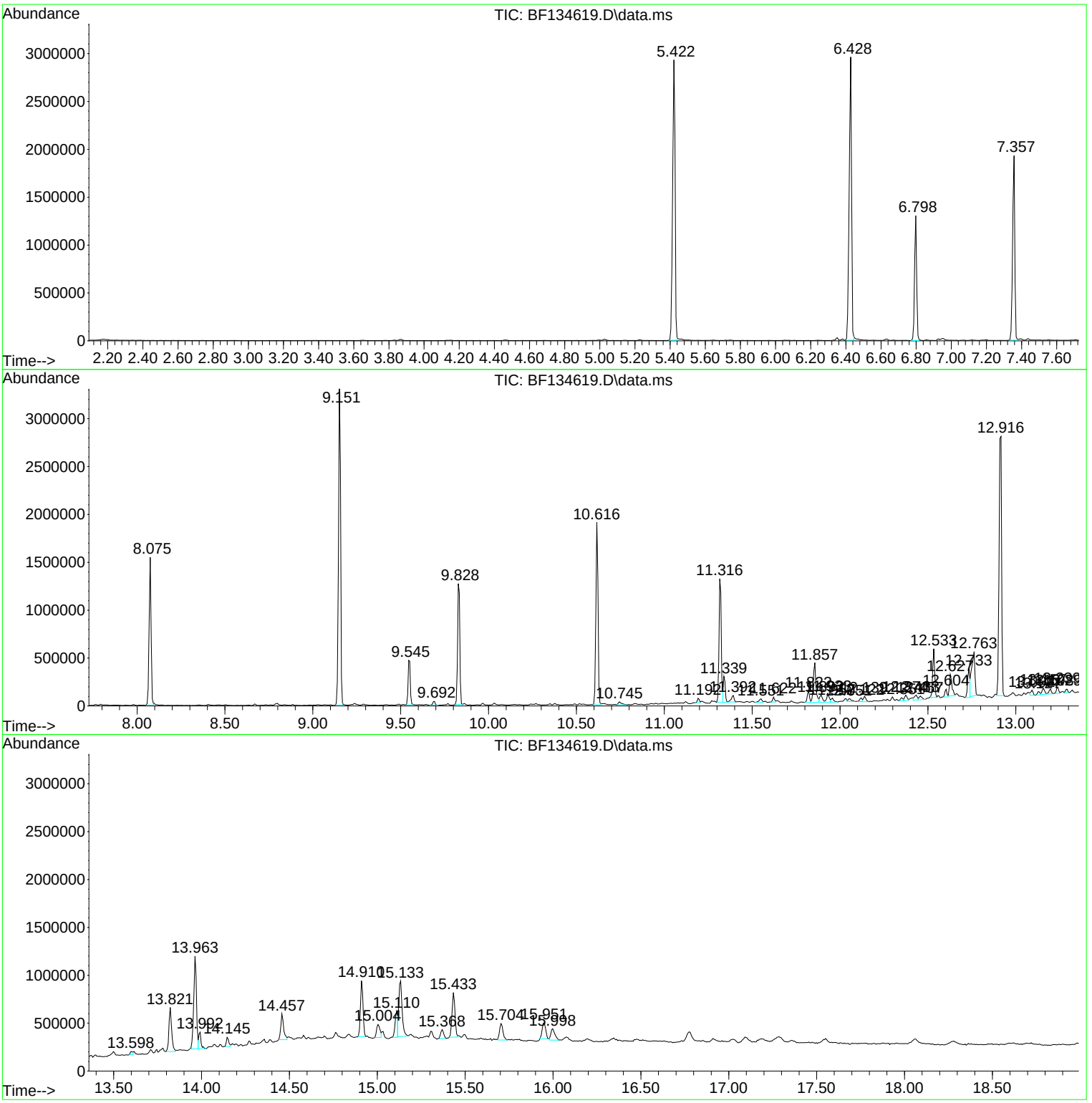
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-0-2-20230721

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080323\
Data File : BF134618.D
Acq On : 03 Aug 2023 18:53
Operator : CG\JU
Sample : 03686-09
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BNA_F
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SB-29-0-2-20230721

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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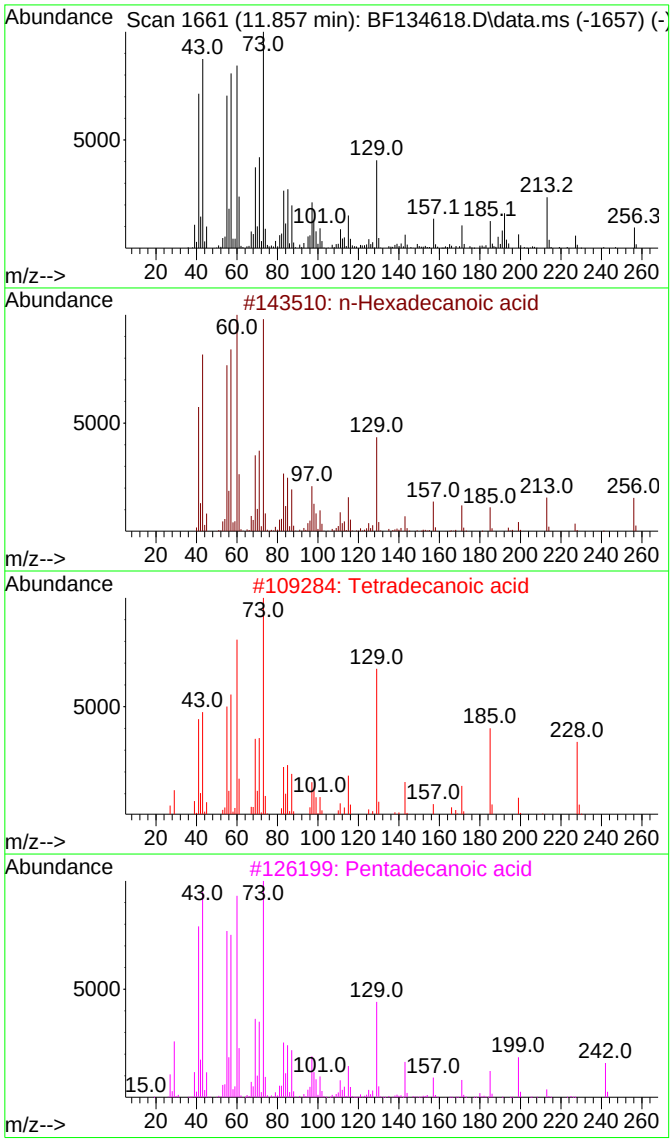
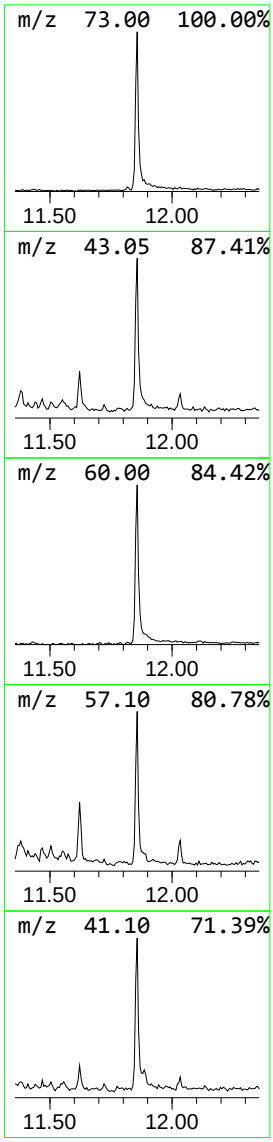
Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	7.32 ng	426726	Phenanthrene-d10	11.316

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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Data File : BF134618.D
Acq On : 03 Aug 2023 18:53
Operator : CG\JU
Sample : 03686-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-0-2-20230721

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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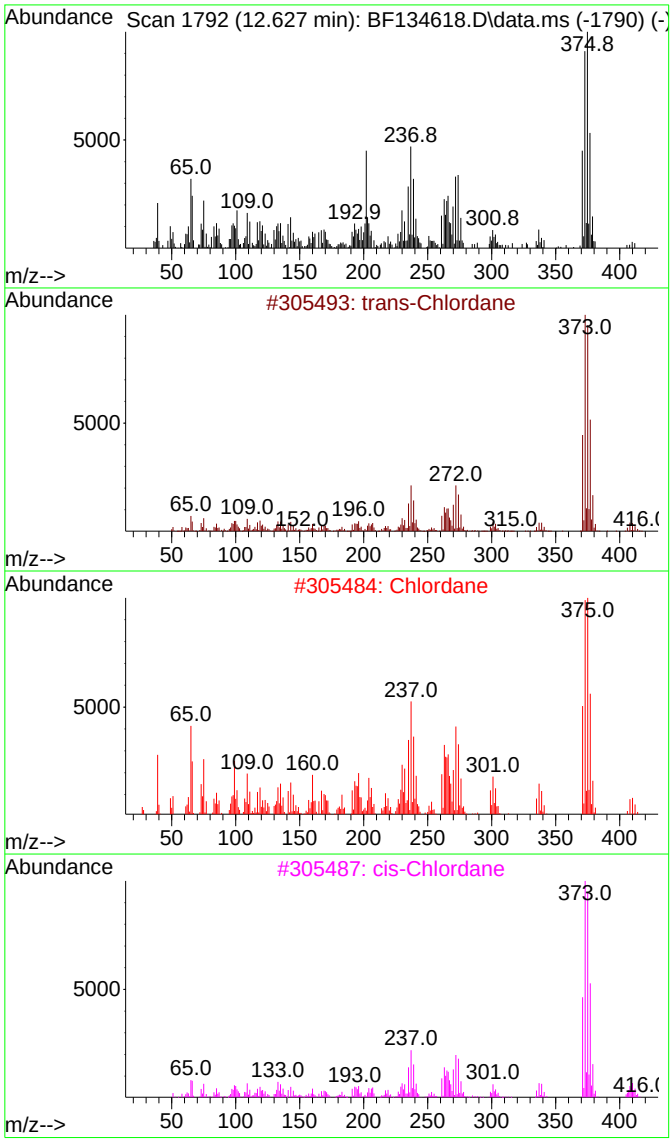
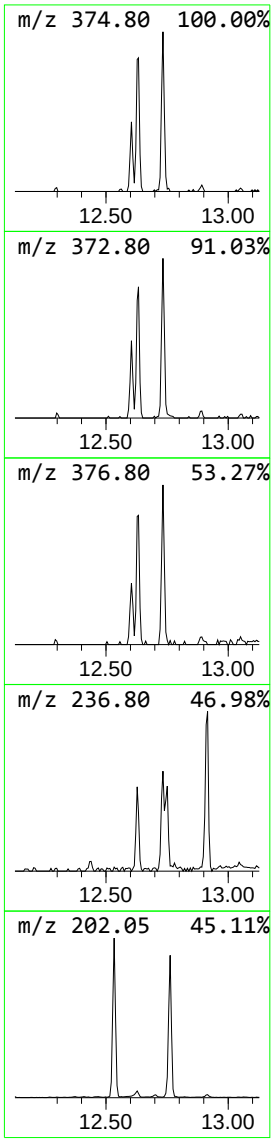
Peak Number 2 trans-Chlordane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	3.79 ng	221149	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Chlordane	406	C10H6Cl8	005103-74-2	95
2	Chlordane	406	C10H6Cl8	000057-74-9	83
3	cis-Chlordane	406	C10H6Cl8	005103-71-9	74
4	4,7-Methanoindene, 1,2,3,5,6,7,8...	406	C10H6Cl8	1000017-10-9	70
5	2,5-Difluorobenzamide, N-(2-iodo...	373	C14H10F2INO	1000358-05-2	10





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Data File : BF134618.D
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Operator : CG\JU
Sample : 03686-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-0-2-20230721

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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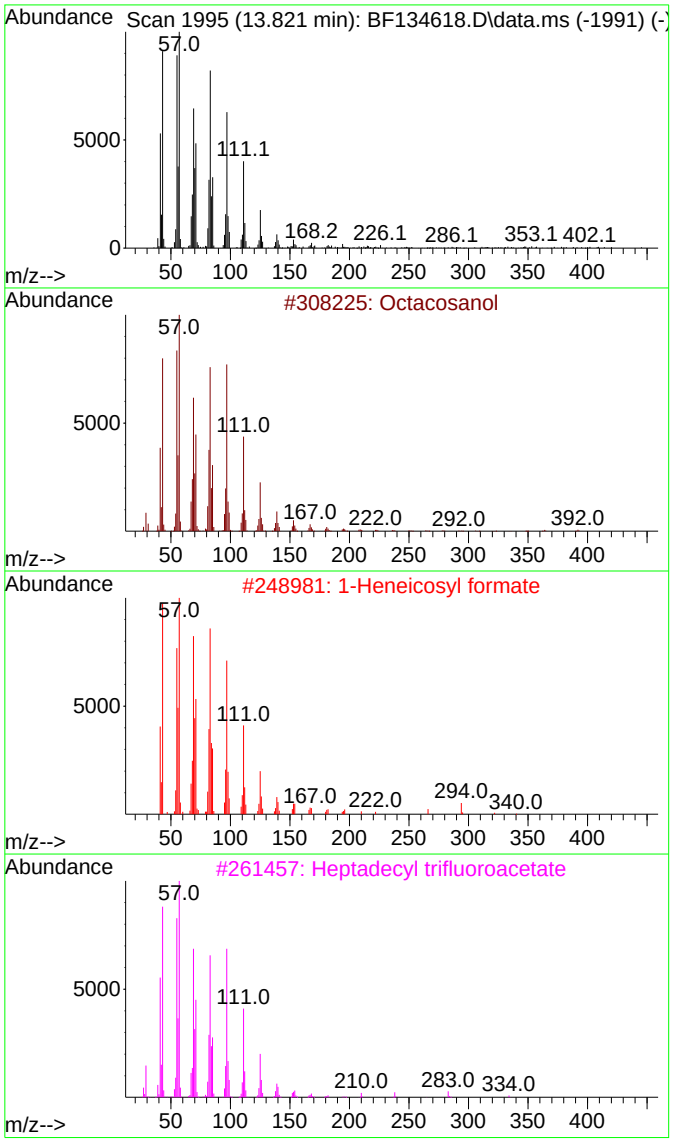
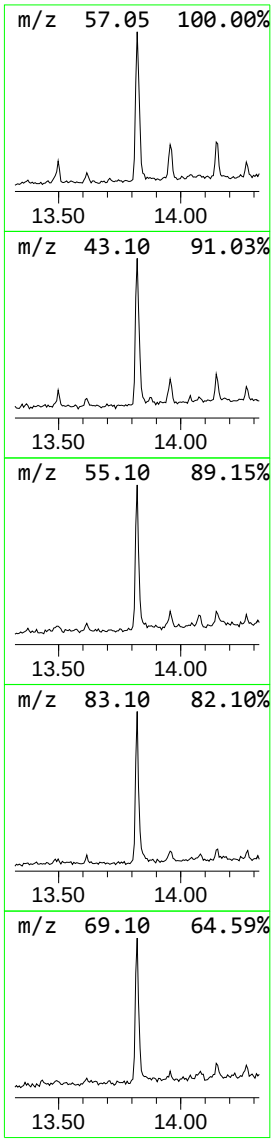
Peak Number 3 Octacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	9.39 ng	495064	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5	1-Hexacosene	364	C26H52	018835-33-1	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080323\
Data File : BF134618.D
Acq On : 03 Aug 2023 18:53
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Sample : 03686-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-0-2-20230721

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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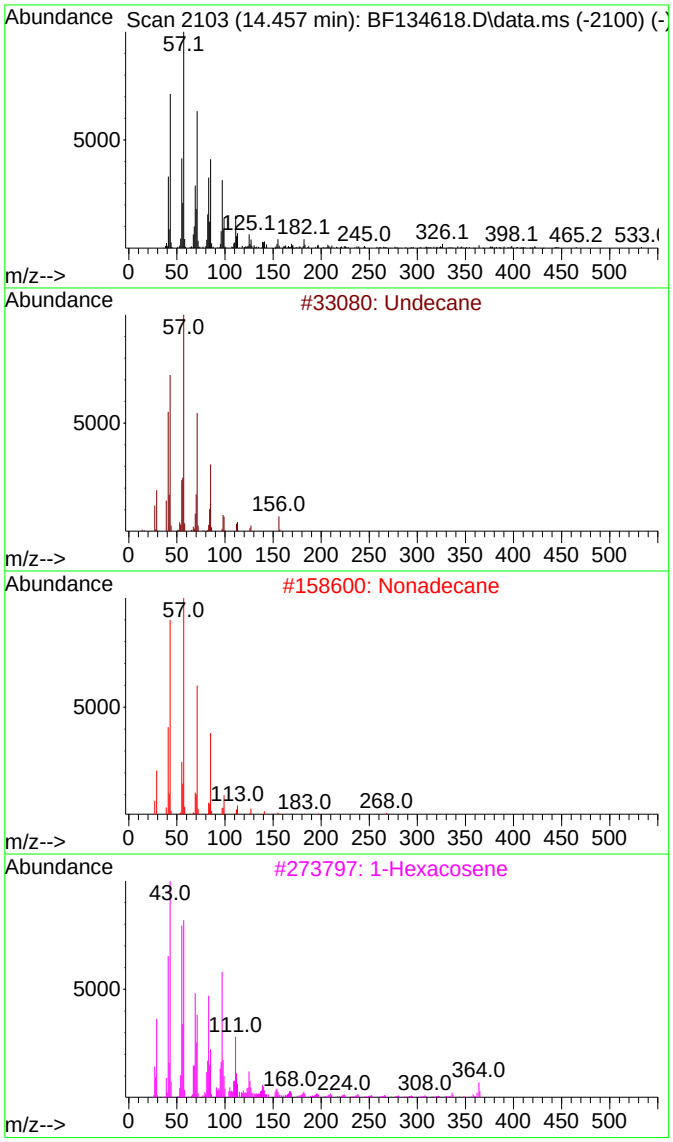
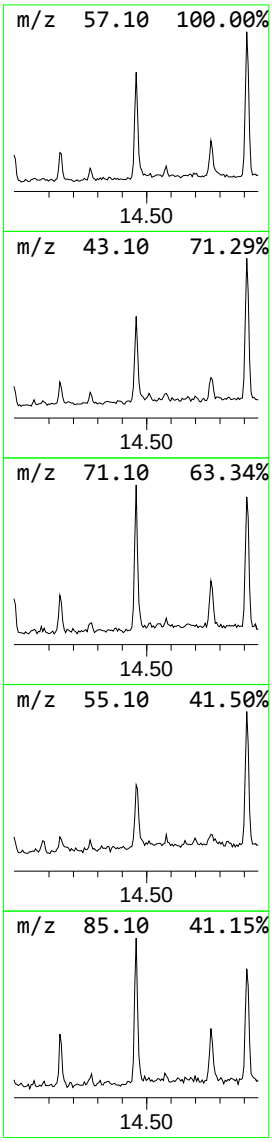
Peak Number 4 Undecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	5.74 ng	302699	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	94
2	Nonadecane	268	C19H40	000629-92-5	93
3	1-Hexacosene	364	C26H52	018835-33-1	93
4	Dodecane	170	C12H26	000112-40-3	93
5	Octacosane	394	C28H58	000630-02-4	92





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080323\
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Operator : CG\JU
Sample : 03686-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-0-2-20230721

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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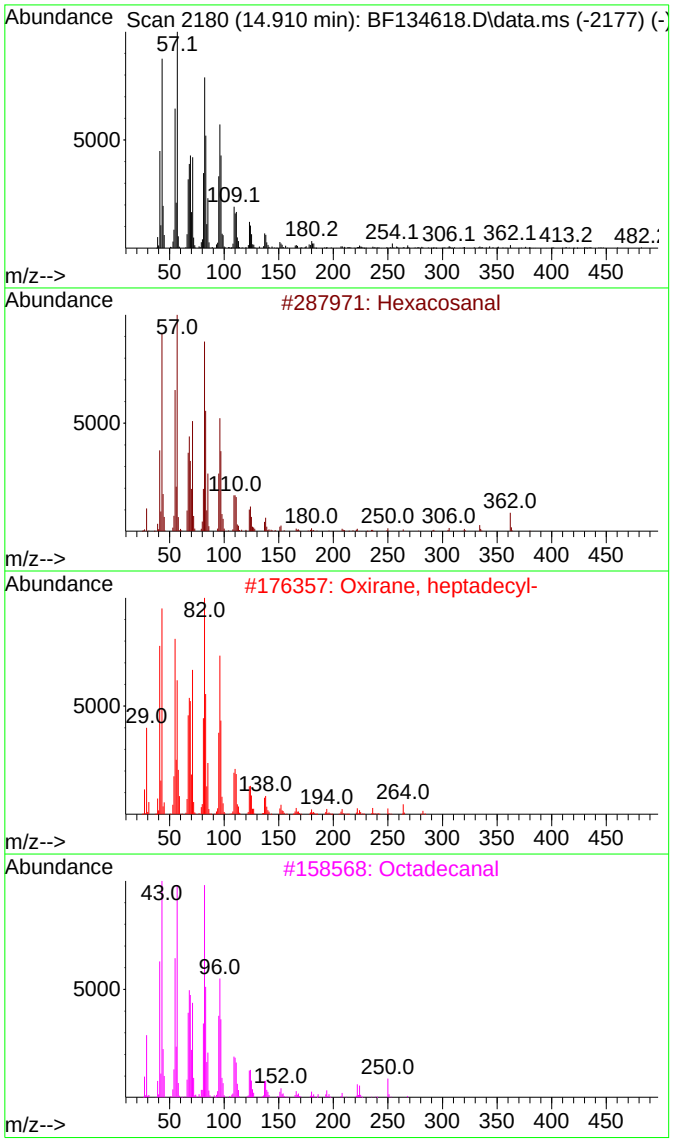
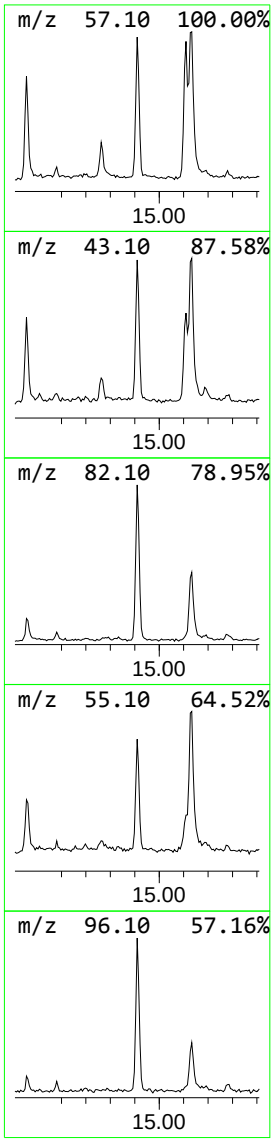
Peak Number 5 Hexacosanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.910	22.03 ng	583047	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosanal	380	C26H52O	026627-85-0	97
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	96
3	Octadecanal	268	C18H36O	000638-66-4	95
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	93
5	Eicosanal-	296	C20H40O	002400-66-0	93





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Instrument :
BNA_F
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SB-29-0-2-20230721

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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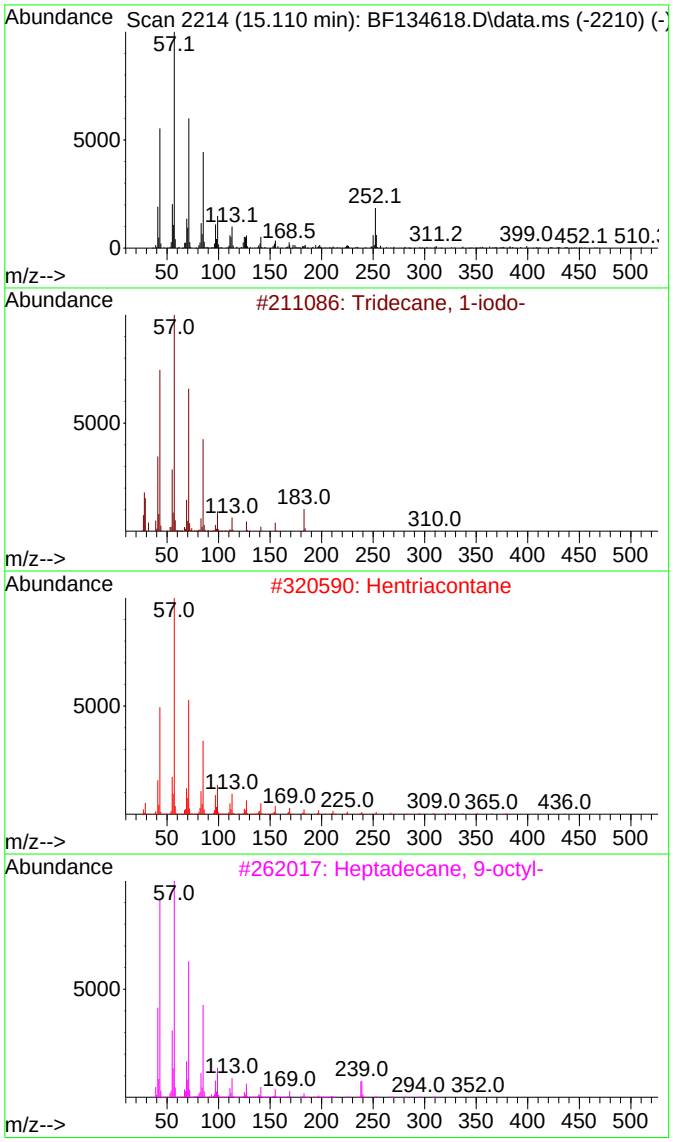
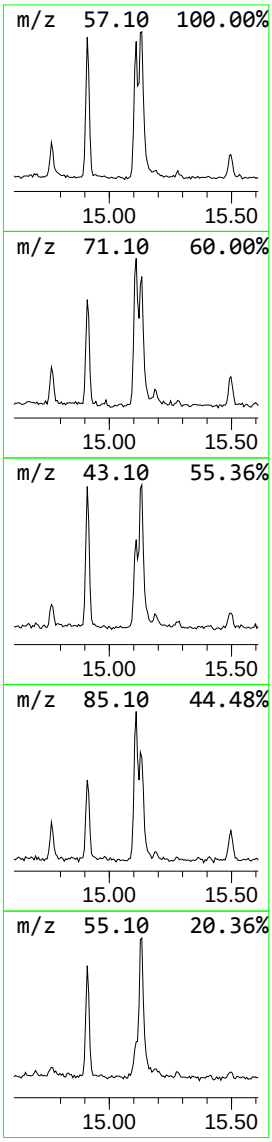
Peak Number 6 Tridecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.110	10.78 ng	285210	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
4	Pentacosane	352	C25H52	000629-99-2	83
5	Hexacosane	366	C26H54	000630-01-3	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080323\
Data File : BF134618.D
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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-0-2-20230721

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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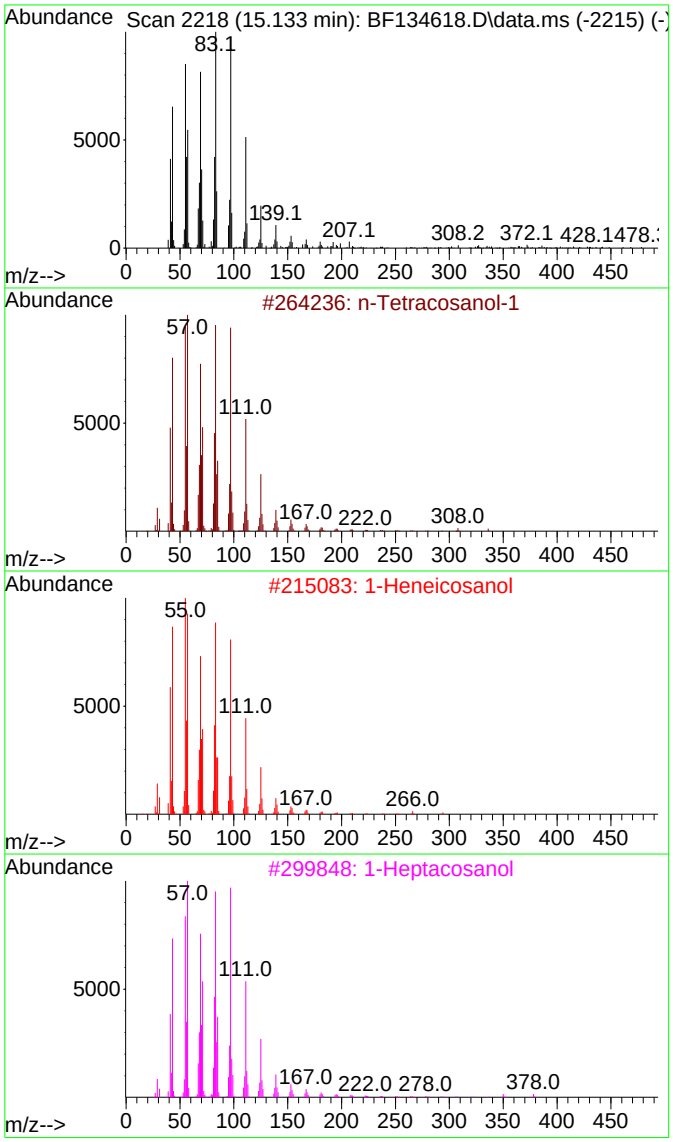
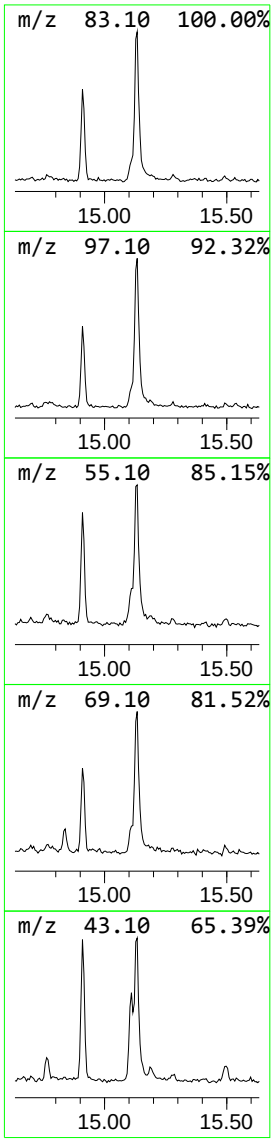
Peak Number 7 n-Tetracosanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	27.58 ng	730040	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	90
4	Eicosyl methyl ether	312	C21H44O	1000406-29-4	90
5	1-Hexacosene	364	C26H52	018835-33-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080323\
Data File : BF134618.D
Acq On : 03 Aug 2023 18:53
Operator : CG\JU
Sample : 03686-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-0-2-20230721

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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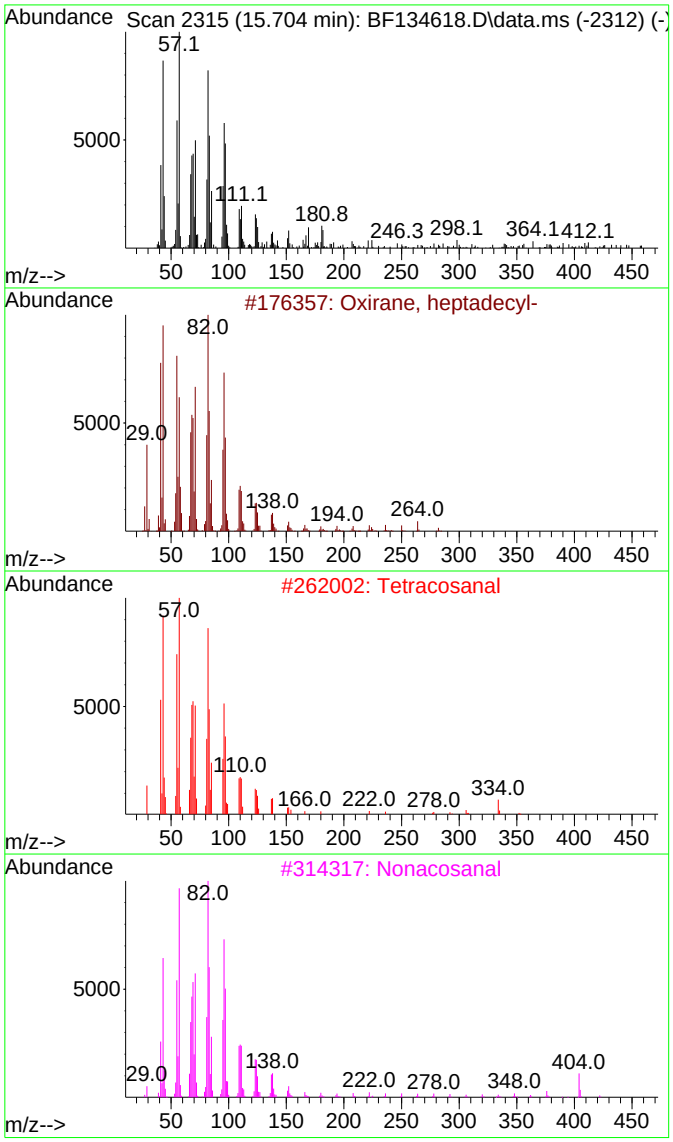
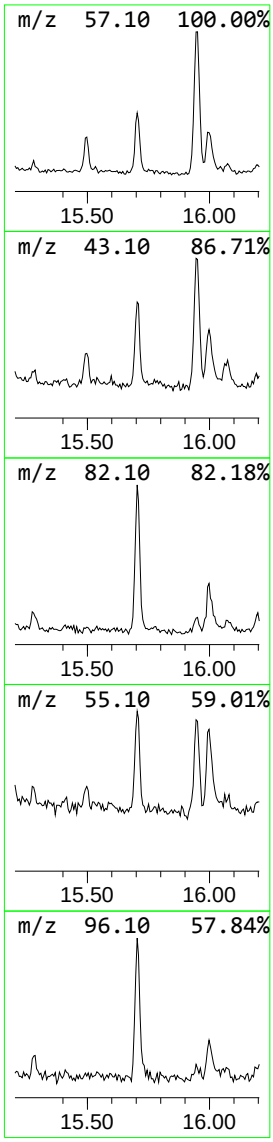
Peak Number 8 Oxirane, heptadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.704	8.63 ng	228474	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2	Tetracosanal	352	C24H48O	057866-08-7	95
3	Nonacosanal	422	C29H58O	072934-04-4	93
4	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	89
5	Octacosanal	408	C28H56O	022725-64-0	87





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Acq On : 03 Aug 2023 18:53
Operator : CG\JU
Sample : 03686-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-0-2-20230721

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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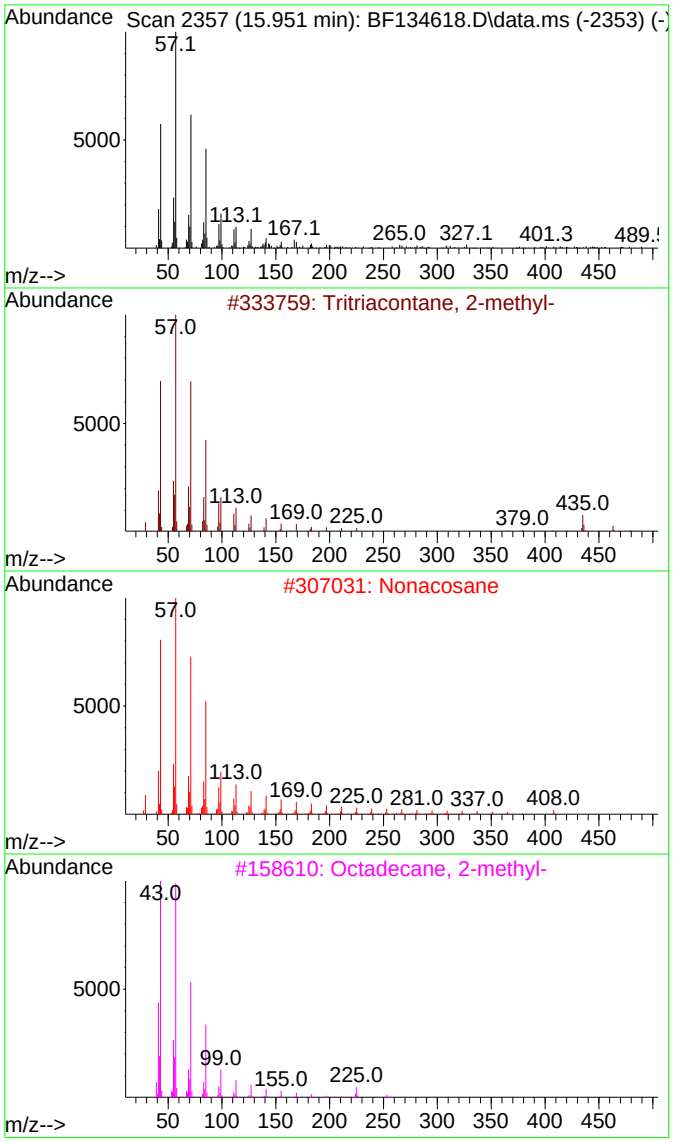
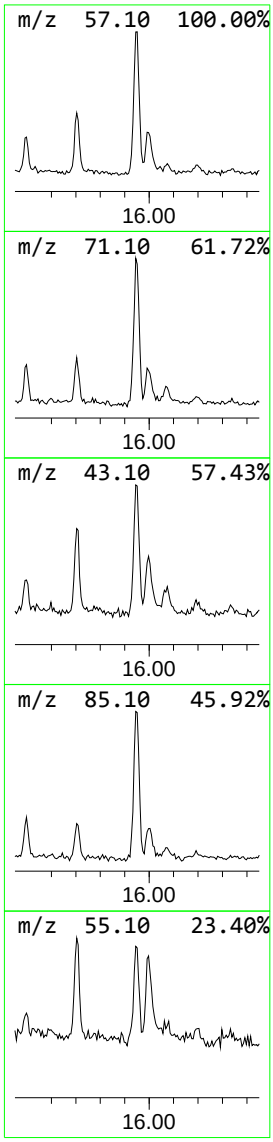
Peak Number 9 Tritriacontane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	8.70 ng	230247	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritriacontane, 2-methyl-	479	C34H70	066214-27-5	98
2	Nonacosane	408	C29H60	000630-03-5	93
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5	4-Methylheneicosane	310	C22H46	025117-29-7	90





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Data File : BF134618.D
Acq On : 03 Aug 2023 18:53
Operator : CG\JU
Sample : 03686-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-0-2-20230721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

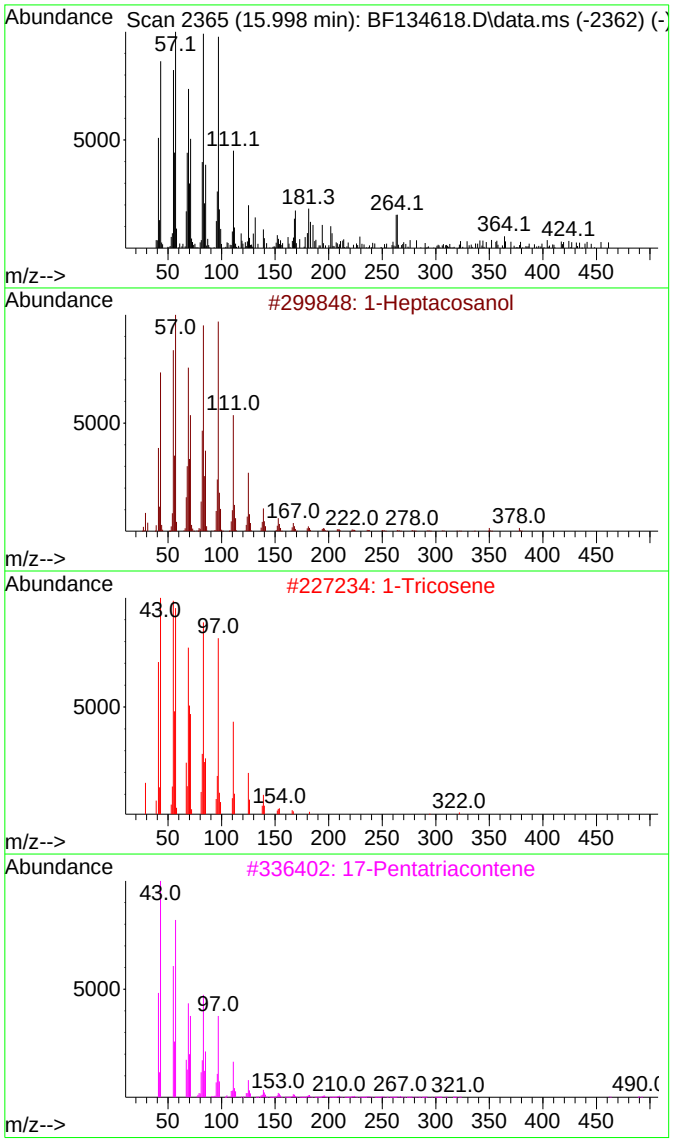
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

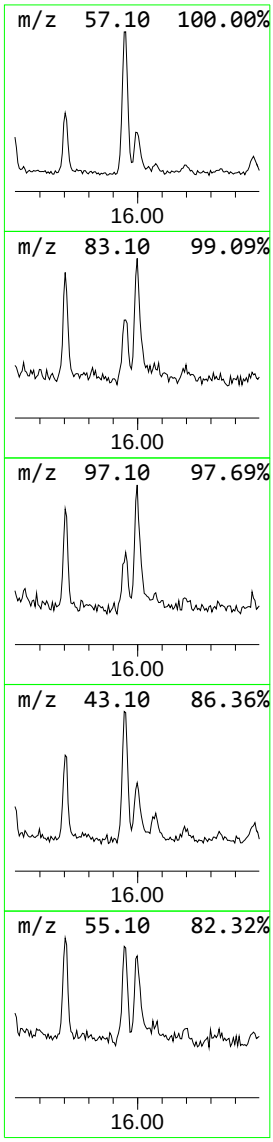
****

Peak Number 10 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	6.95 ng	183819	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	1-Tricosene	322	C23H46	018835-32-0	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	90
4	Octacosyl acetate	452	C30H60O2	018206-97-8	89
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080323\
Data File : BF134618.D
Acq On : 03 Aug 2023 18:53
Operator : CG\JU
Sample : 03686-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-0-2-20230721

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	11.857	7.3	ng	426726	4	11.316	1165590	20.0
trans-Chlordane	12.627	3.8	ng	221149	4	11.316	1165590	20.0
Octacosanol	13.821	9.4	ng	495064	5	13.963	1054650	20.0
Undecane	14.457	5.7	ng	302699	5	13.963	1054650	20.0
Hexacosanal	14.910	22.0	ng	583047	6	15.433	529329	20.0
Tridecane, 1-iodo-	15.110	10.8	ng	285210	6	15.433	529329	20.0
n-Tetracosanol-1	15.133	27.6	ng	730040	6	15.433	529329	20.0
Oxirane, heptad...	15.704	8.6	ng	228474	6	15.433	529329	20.0
Tritriacontane,...	15.951	8.7	ng	230247	6	15.433	529329	20.0
1-Heptacosanol	15.998	7.0	ng	183819	6	15.433	529329	20.0