LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

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-BF083023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135020.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	7	11	19	rVB2	39613	57564	2.08%	0.261%
2	5.004	492	496	503	rVB	89545	111097	4.01%	0.503%
3	5.404	559	564	567	rBV	2857623	2669773	96.27%	12.083%
4	6.410	730	735	738	rBV	2748665	2678660	96.59%	12.123%
5	6.769	793	796	800	rBV	965806	788171	28.42%	3.567%
6	7.334	887	892	895	rBV	1827184	1690722	60.96%	7.652%
7	8.051	1009	1014	1017	rBV	1251085	1063873	38.36%	4.815%
8	9.128	1192	1197	1201	rBV	2963202	2773301	100.00%	12.551%
9	9.251	1214	1218	1220	rBV	32872	30034	1.08%	0.136%
10	9.810	1308	1313	1316	rBV	1269335	1133026	40.85%	5.128%
11	10.598	1443	1447	1451	rBV	1844170	1588266	57.27%	7.188%
12	11.298	1562	1566	1569	rBV	1202426	1046510	37.74%	4.736%
13	11.322	1569	1570	1574	rVV	151357	94404	3.40%	0.427%
14	11.374	1574	1579	1582	rVB	26236	28487	1.03%	0.129%
15	11.804	1649	1652	1654	rBV	29094	28627	1.03%	0.130%
16	11.839	1654	1658	1668	rVB2	529319	533978	19.25%	2.417%
17	11.916	1668	1671	1673	rBV2	34253	30042	1.08%	0.136%
18	12.516	1769	1773	1777	rBV	287675	249026	8.98%	1.127%
19	12.627	1787	1792	1805	rBV2	186082	222943	8.04%	1.009%
20	12.745	1806	1812	1816	rBV	216994	219409	7.91%	0.993%
21	12.898	1834	1838	1841	rBV	2234086	1886399	68.02%	8.537%
22	12.968	1844	1850	1853	rBV3	18664	33774	1.22%	0.153%
23	13.080	1866	1869	1872	rVB3	32727	33730	1.22%	0.153%
24	13.145	1877	1880	1883	rVB2	31465	34698	1.25%	0.157%
25	13.486	1931	1938	1940	rBV4	25699	40364	1.46%	0.183%
26	13.698	1971	1974	1977	rBV2	22905	29012	1.05%	0.131%
27	13.810	1989	1993	2002	rBV2	151333	206386	7.44%	0.934%
28	13.957	2012	2018	2020	rBV2	724084	786835	28.37%	3.561%
29	13.980	2020	2022	2025	rVB	103791	84179	3.04%	0.381%
30	14.445	2097	2101	2107	rBV6	45543	93842	3.38%	0.425%
31	14.727	2146	2149	2151	rBV2	28587	31500	1.14%	0.143%
32	14.898	2174	2178	2182	rBV	103727	117353	4.23%	0.531%
33	14.992	2190	2194	2198	rBV	106165	167248	6.03%	0.757%
34	15.092	2207	2211	2213	rBV	58209	72544	2.62%	0.328%
35	15.121	2213	2216	2223	rVB2	62258	105642	3.81%	0.478%
36	15.298	2242	2246	2253	rVB	64325	83218	3.00%	0.377%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

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-BF083023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.357	2253	2256	2262	rBV	84750	107642	3.88%	0.487%
38	15.421	2262	2267	2272	rBV	558572	722064	26.04%	3.268%
39	15.680	2308	2311	2316	rVB4	29637	42693	1.54%	0.193%
40	15.915	2347	2351	2357	rBV	66747	103800	3.74%	0.470%
41	15.980	2360	2362	2370	rVB6	26766	40074	1.44%	0.181%
42	16.733	2486	2490	2497	rVB7	25536	50632	1.83%	0.229%
43	16.892	2512	2517	2527	rBV3	40169	92667	3.34%	0.419%
44	17.045	2538	2543	2548	rBV5	23962	53980	1.95%	0.244%
45	17.339	2589	2593	2599	rVB	22051	37605	1.36%	0.170%

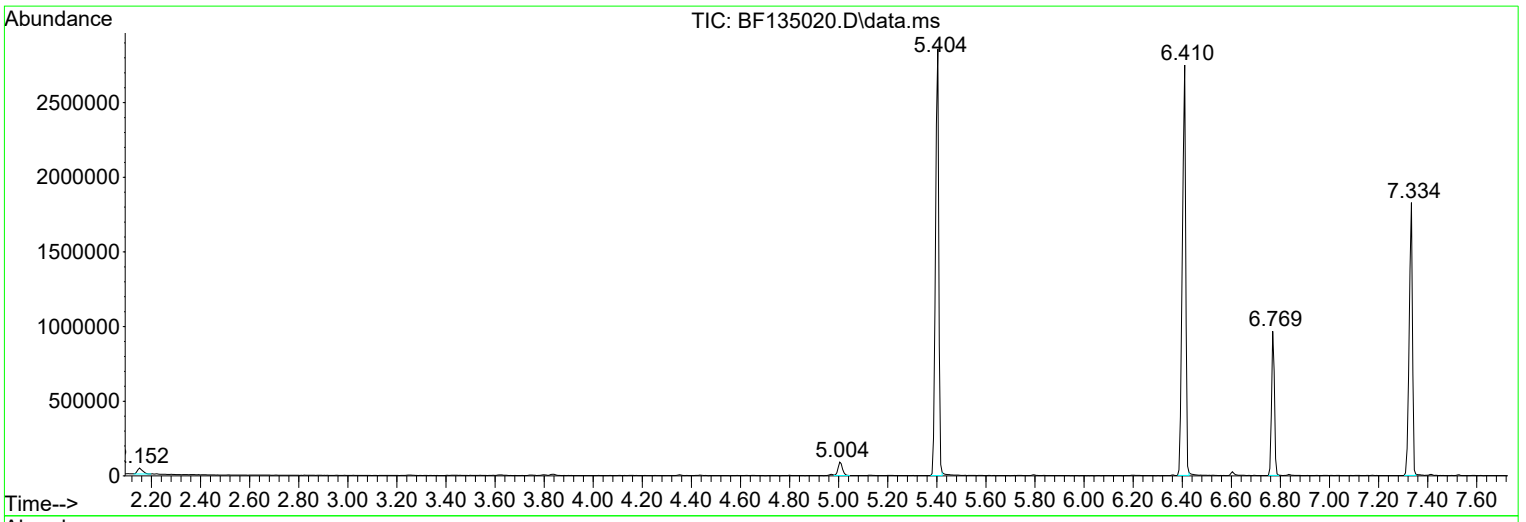
Sum of corrected areas: 22095794

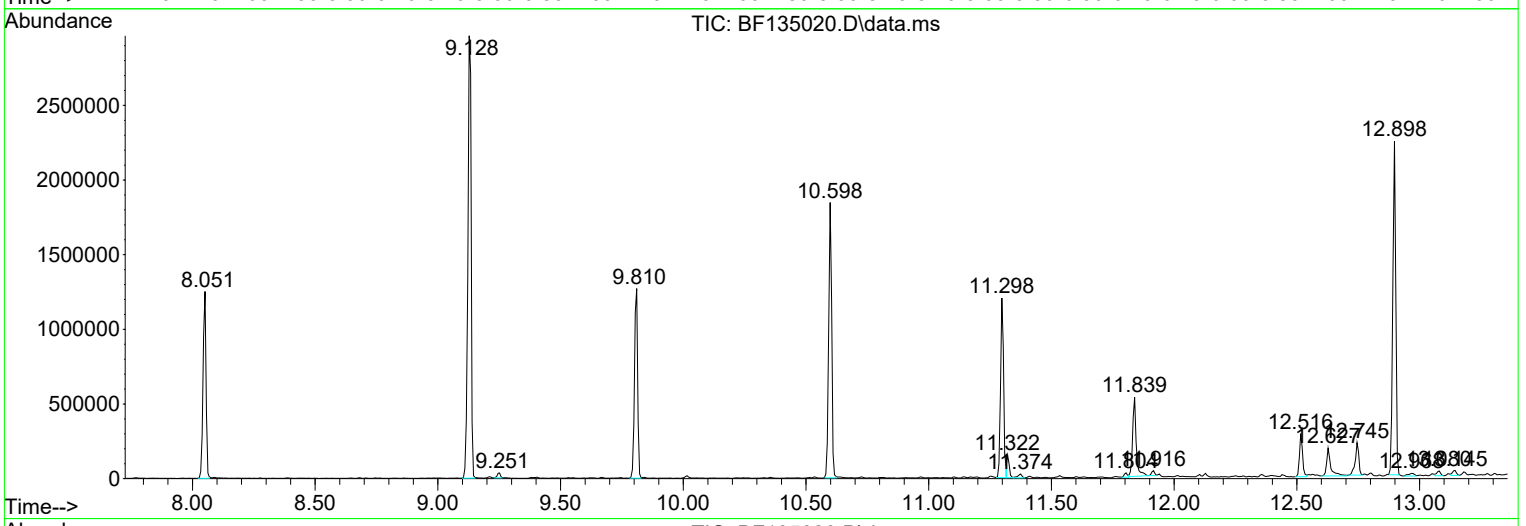
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

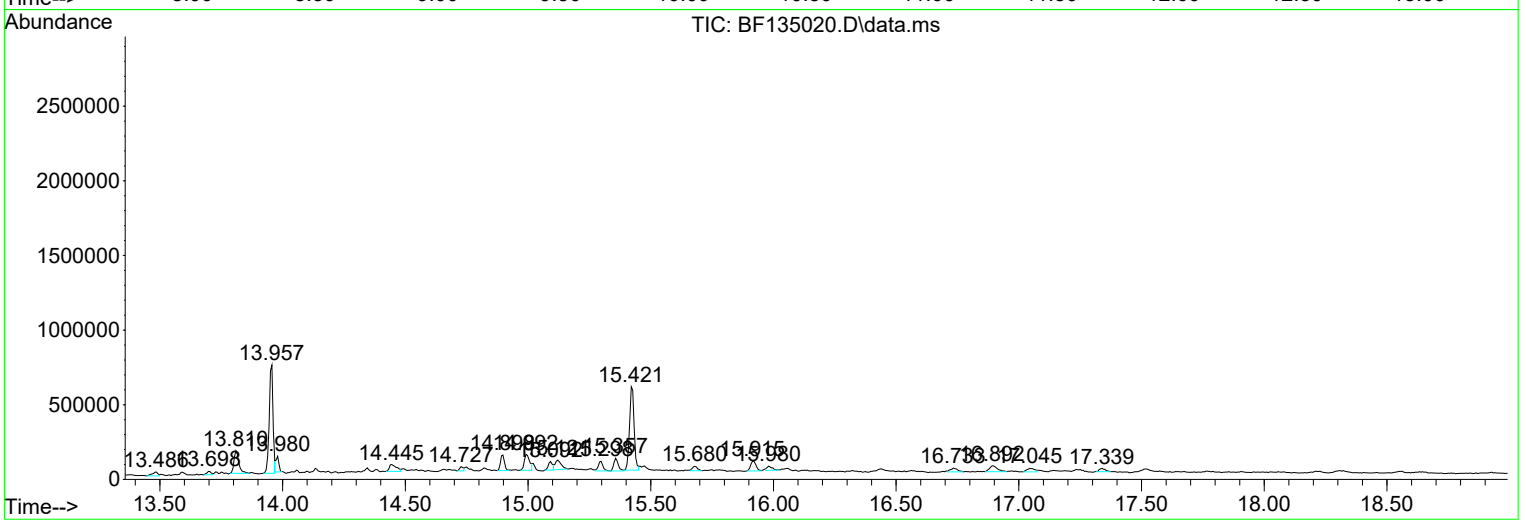
Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

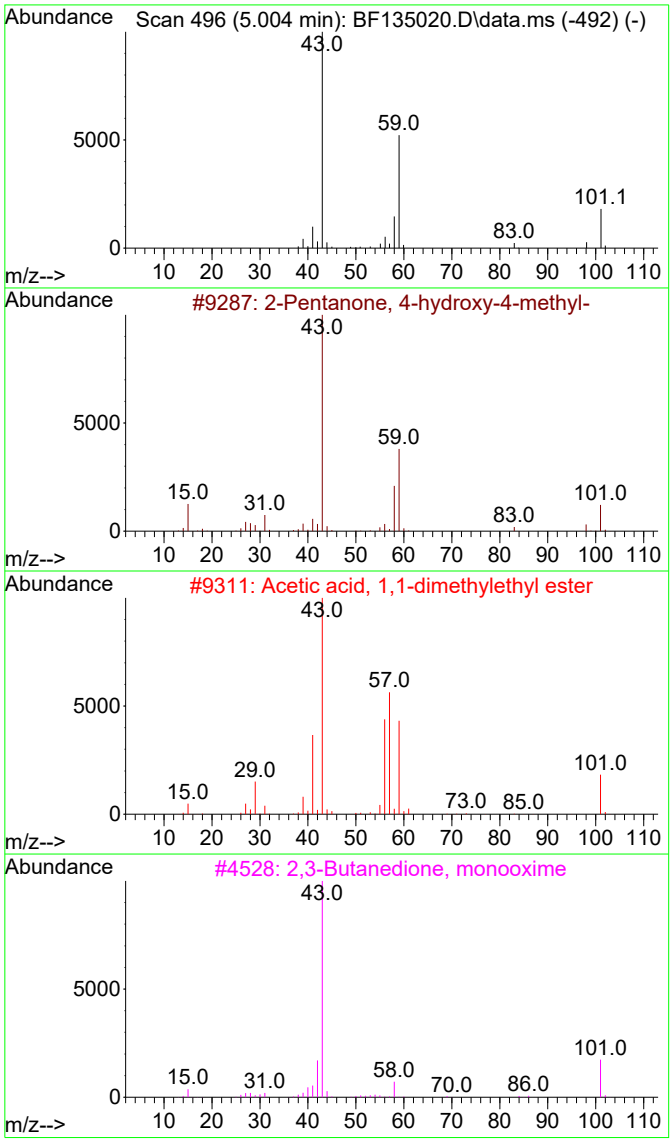
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

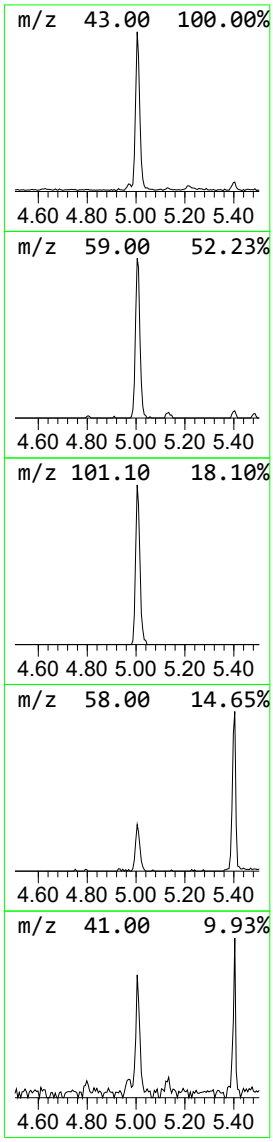
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.82 ng	111097	1,4-Dichlorobenzene-d4	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

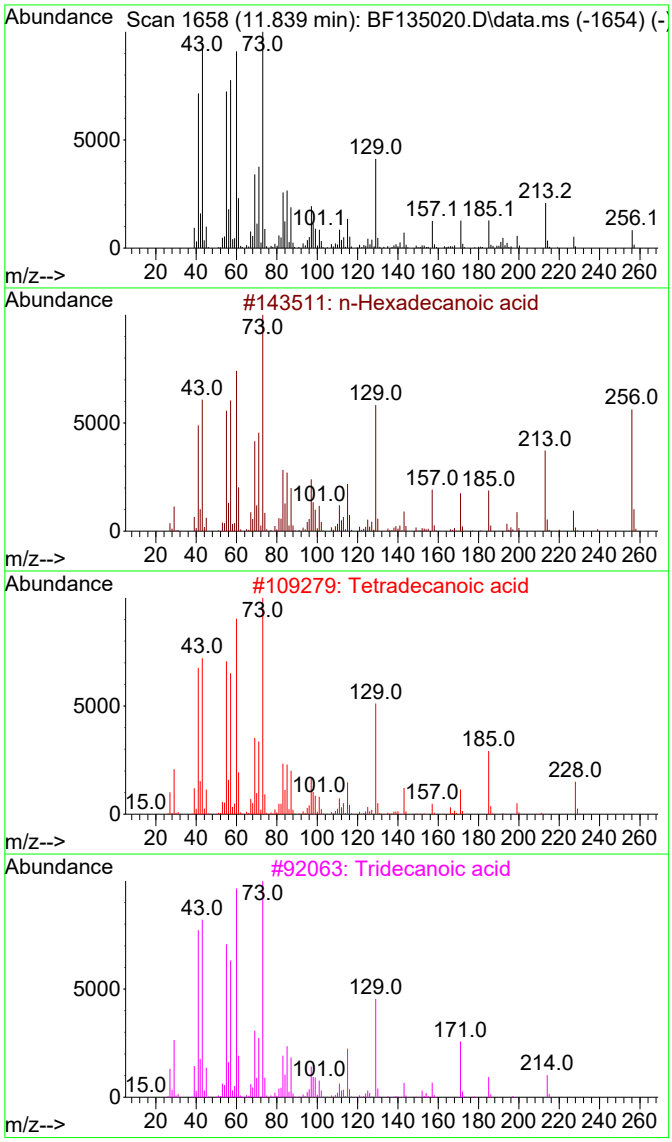
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

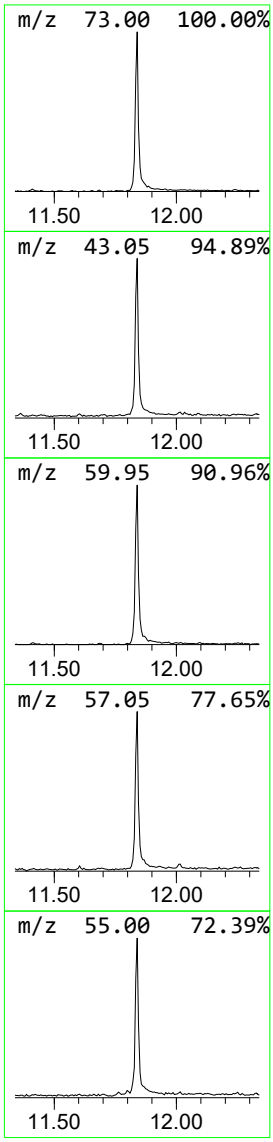
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	10.20 ng	533978	Phenanthrene-d10	11.298

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	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

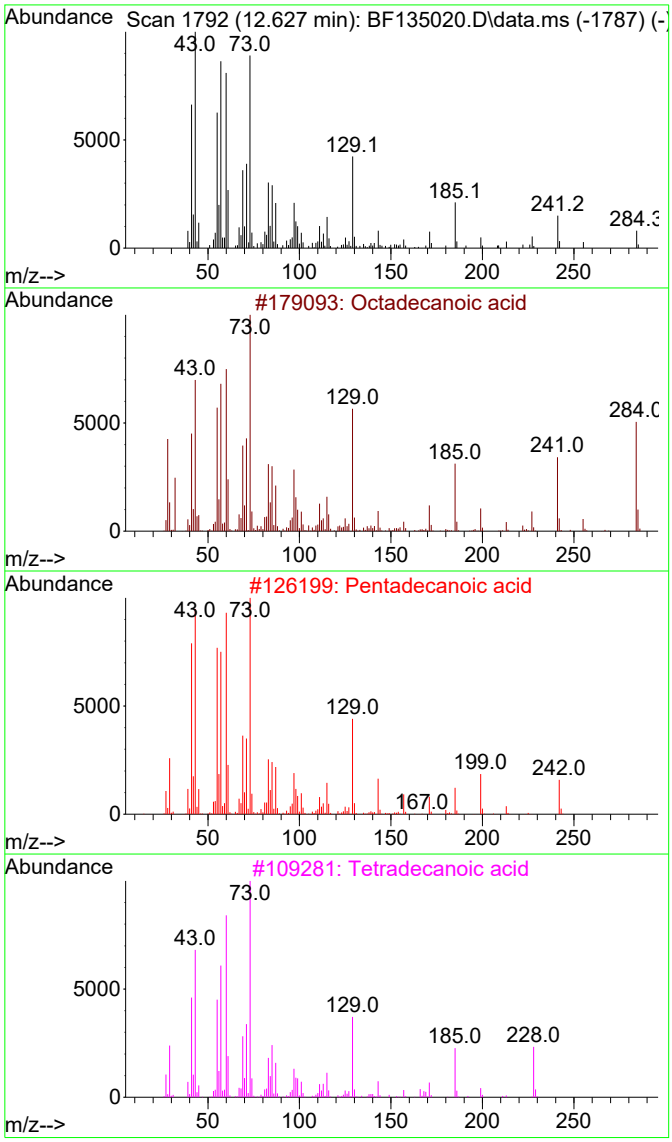
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

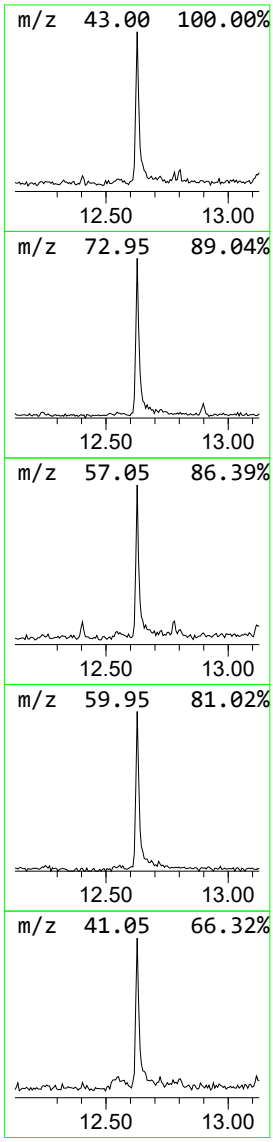
****

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	5.67 ng	222943	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

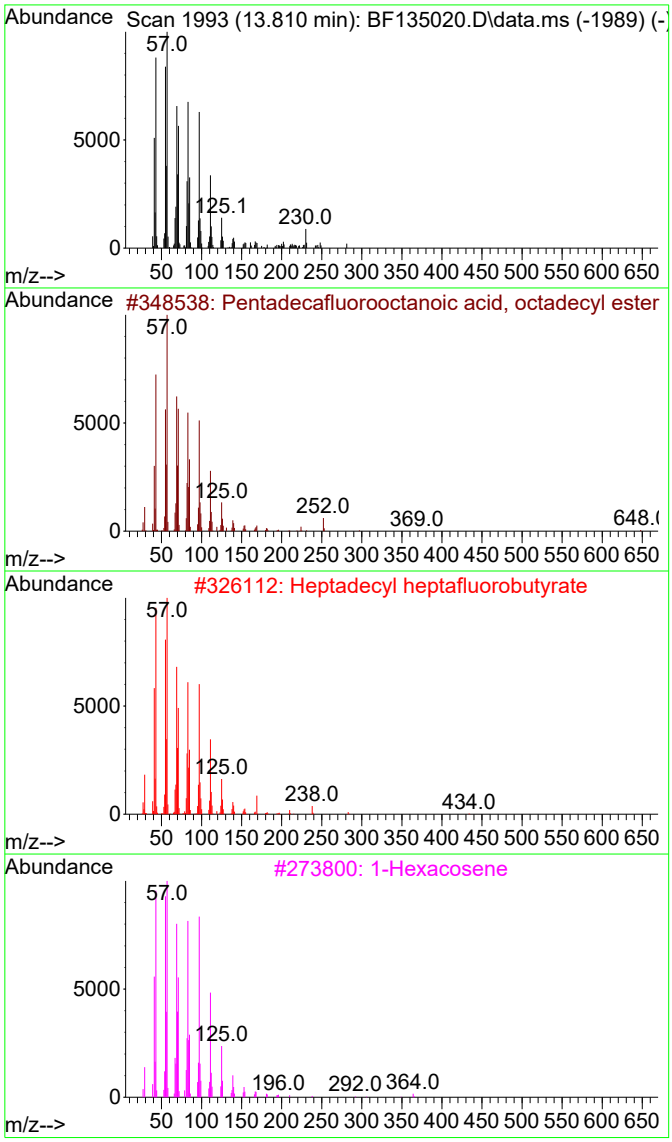
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

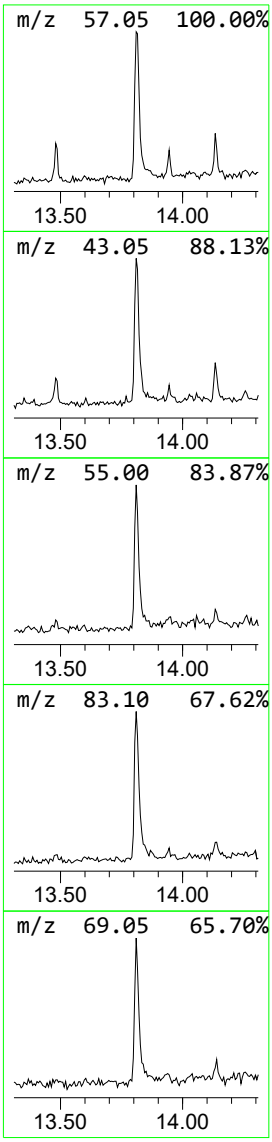
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	5.25 ng	206386	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Hexacosene	364	C26H52	018835-33-1	94
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

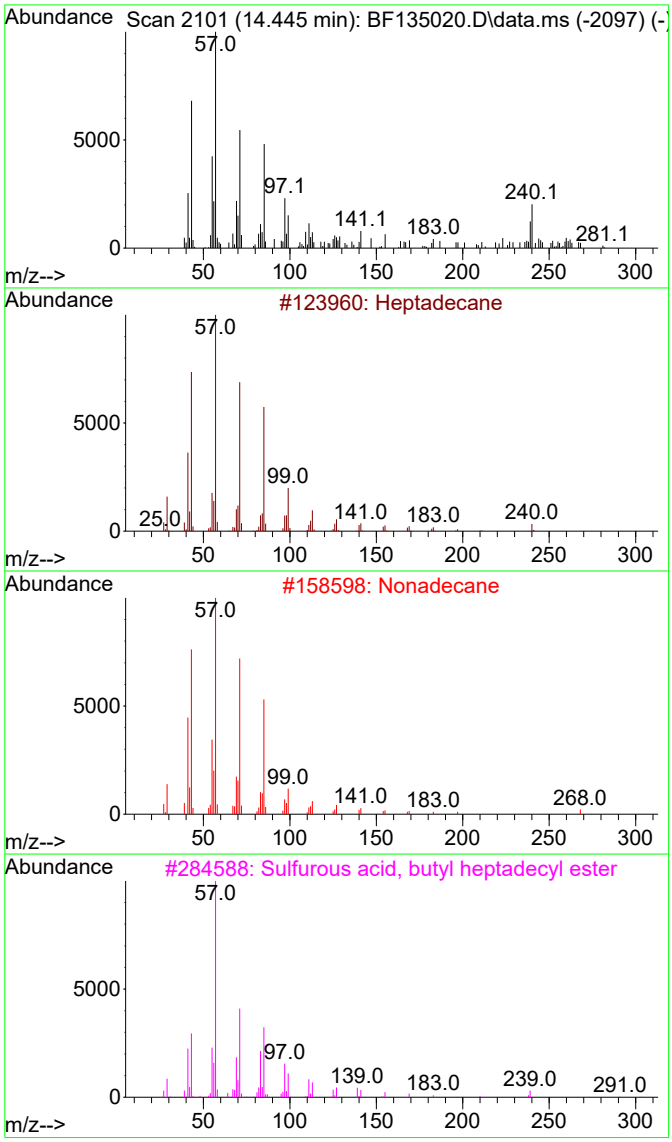
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

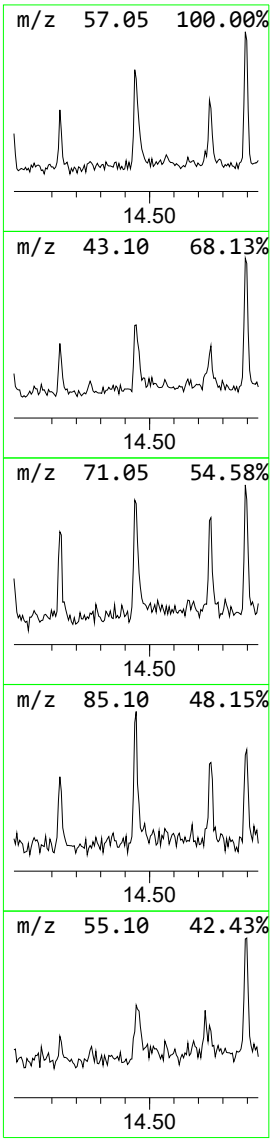
****

Peak Number 5 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	2.39 ng	93842	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Nonadecane	268	C19H40	000629-92-5	87
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	62
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	58
5	10-Methylnonadecane	282	C20H42	056862-62-5	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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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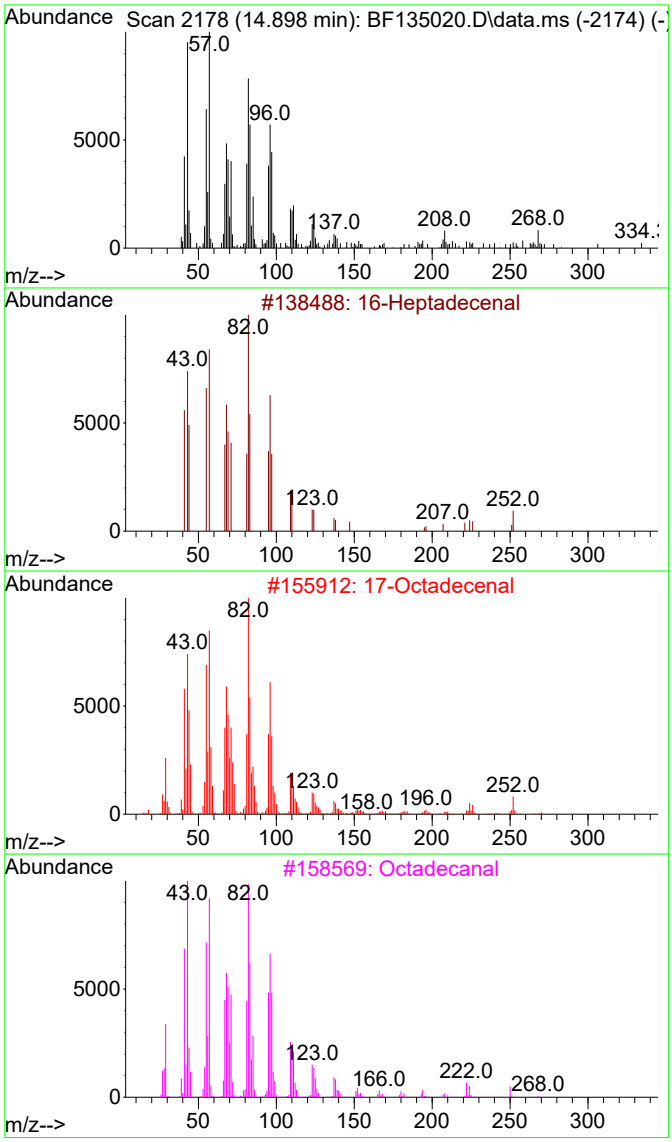
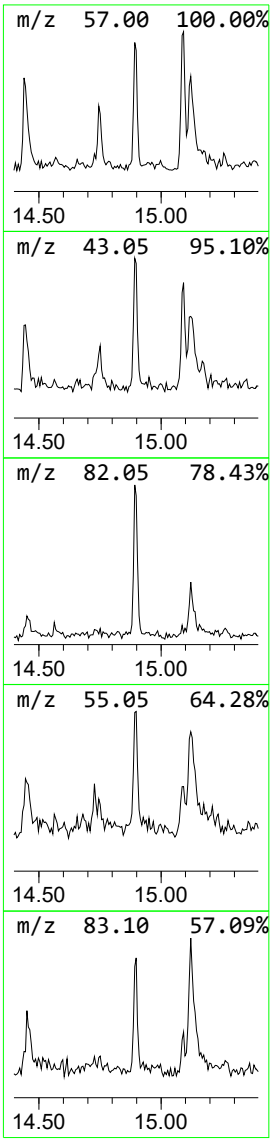
Peak Number 6 16-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	3.25 ng	117353	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Heptadecenal	252	C17H32O	1010144-57-9	93
2	17-Octadecenal	266	C18H34O	056554-86-0	91
3	Octadecanal	268	C18H36O	000638-66-4	90
4	15-Octadecenal	266	C18H34O	056554-93-9	90
5	1,19-Eicosadiene	278	C20H38	014811-95-1	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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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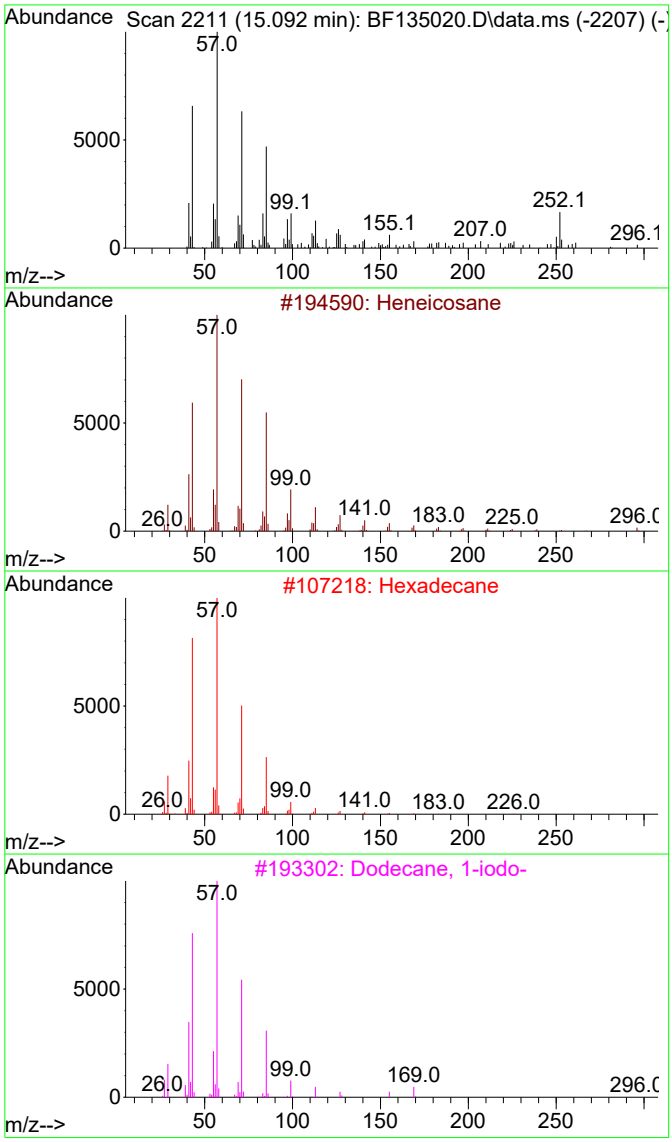
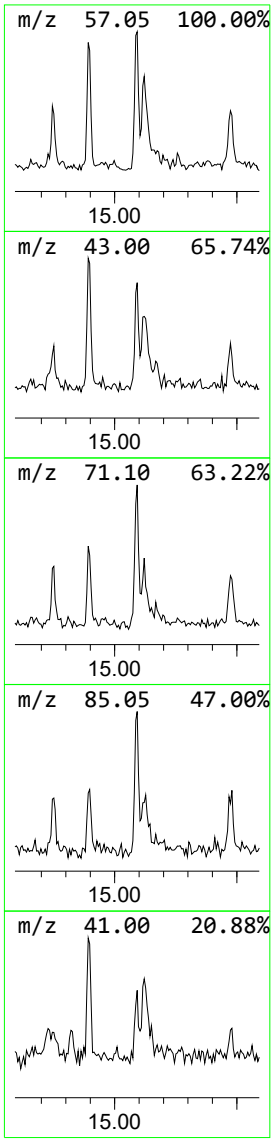
Peak Number 7 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.01 ng	72544	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Hexadecane	226	C16H34	000544-76-3	94
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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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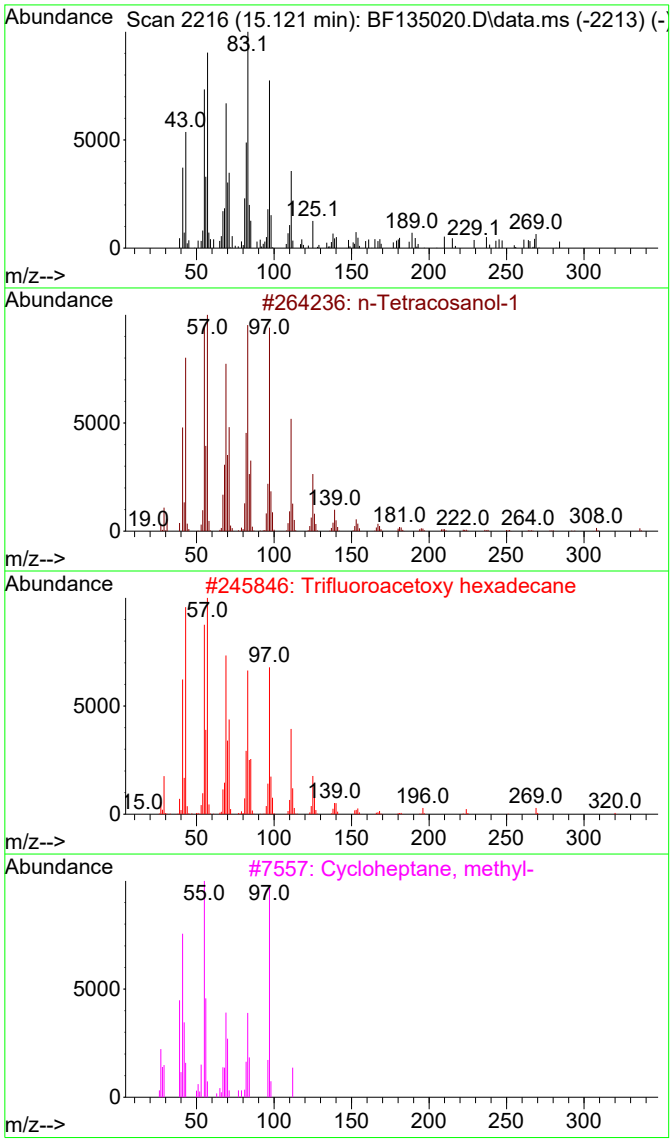
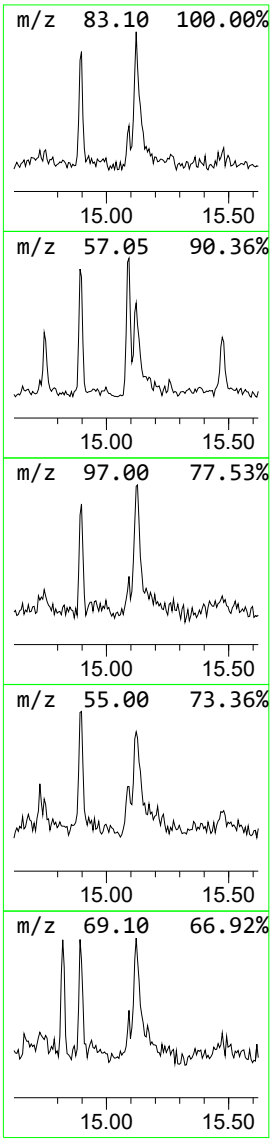
Peak Number 8 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	2.93 ng	105642	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	52
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	52
3	Cycloheptane, methyl-	112	C8H16	004126-78-7	49
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	45
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	45





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Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
OR-345-COMP-01

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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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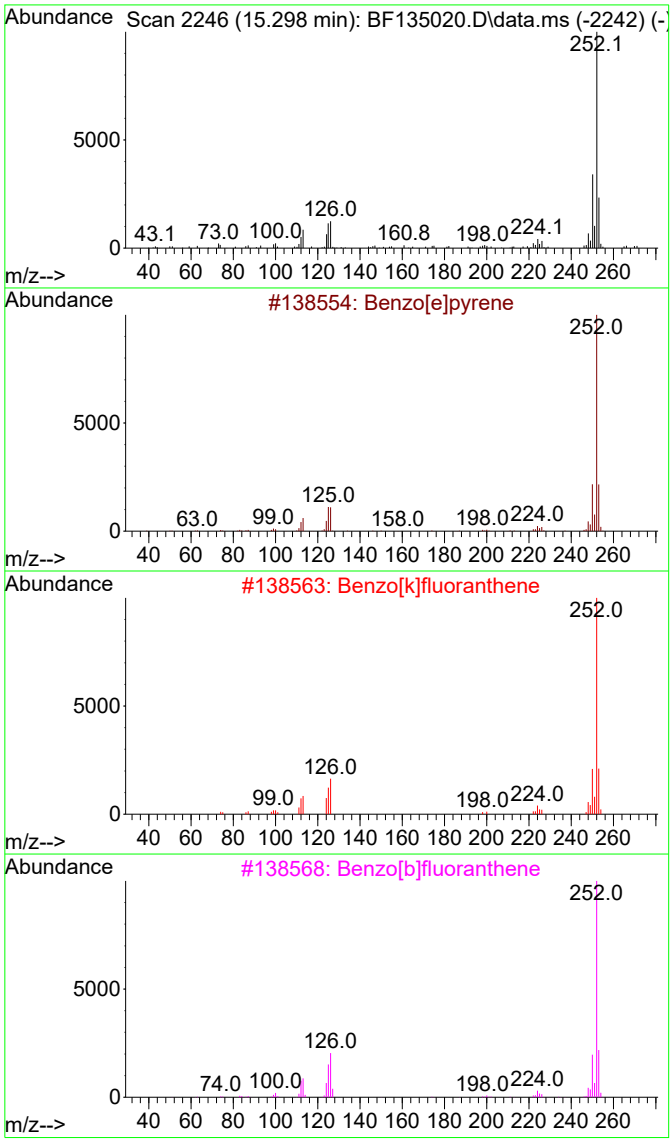
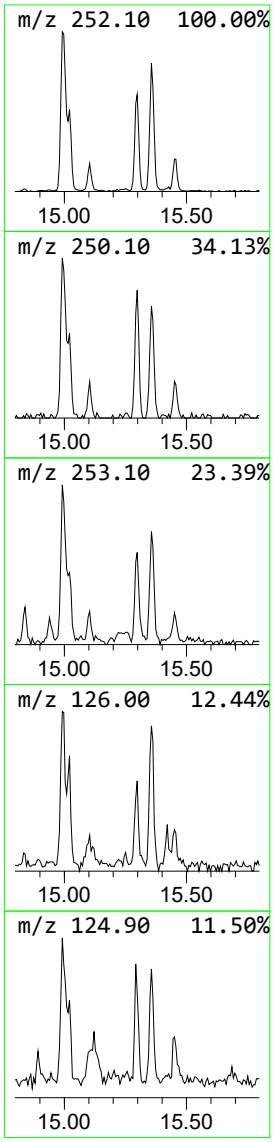
Peak Number 9 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	2.31 ng	83218	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4	Benzo[a]pyrene	252	C20H12	000050-32-8	91
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





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Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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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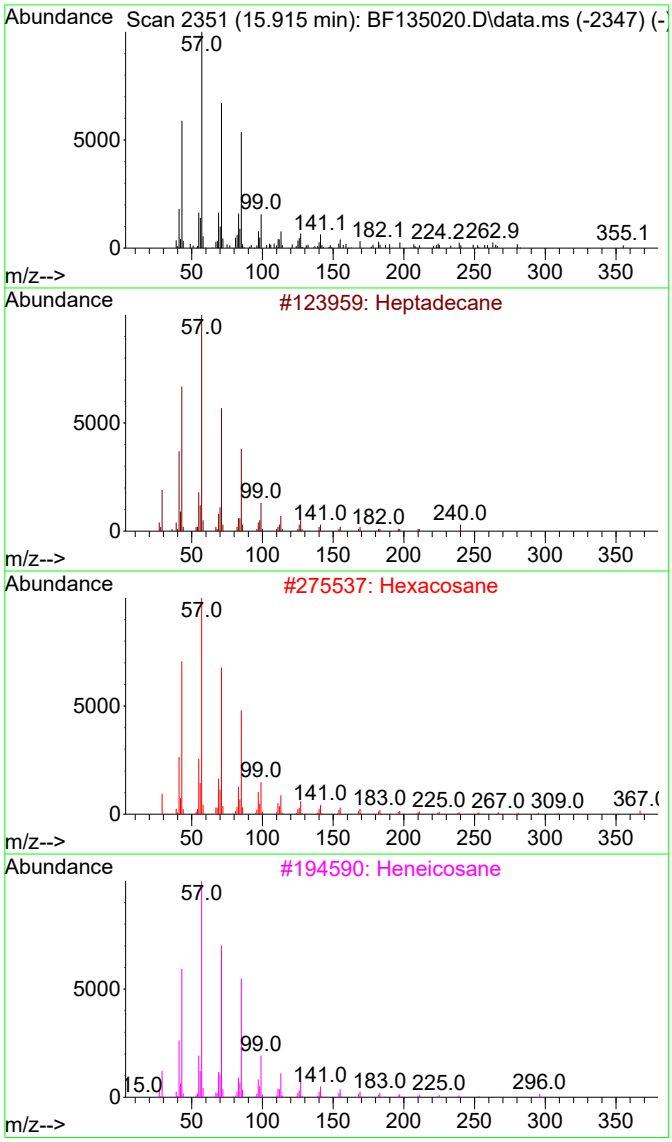
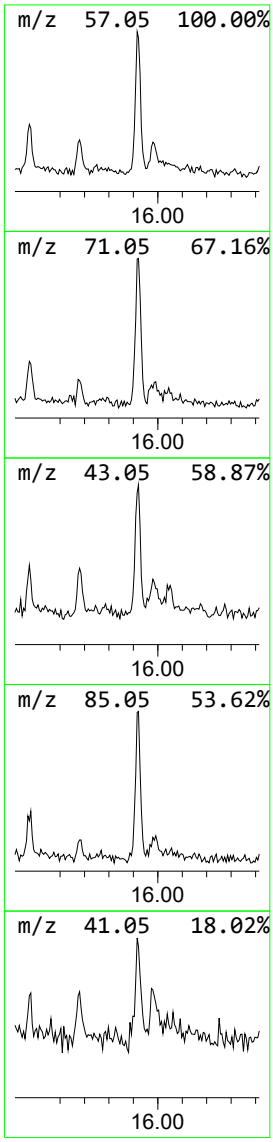
Peak Number 10 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.915	2.88 ng	103800	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	95
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Pentacosane	352	C25H52	000629-99-2	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135020.D
Acq On : 30 Aug 2023 23:44
Operator : CG\JU
Sample : 04196-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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-Pentanone, 4-...	5.004	2.8	ng	111097	1	6.769	788171	20.0
n-Hexadecanoic ...	11.839	10.2	ng	533978	4	11.298	1046510	20.0
Octadecanoic acid	12.627	5.7	ng	222943	5	13.957	786835	20.0
Pentadecafluoro...	13.810	5.3	ng	206386	5	13.957	786835	20.0
Heptadecane	14.445	2.4	ng	93842	5	13.957	786835	20.0
16-Heptadecenal	14.898	3.3	ng	117353	6	15.421	722064	20.0
Heneicosane	15.092	2.0	ng	72544	6	15.421	722064	20.0
n-Tetracosanol-1	15.121	2.9	ng	105642	6	15.421	722064	20.0
Benzo[e]pyrene	15.298	2.3	ng	83218	6	15.421	722064	20.0
Hexacosane	15.915	2.9	ng	103800	6	15.421	722064	20.0