LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137084.D
Acq On : 16 Jan 2024 17:39
Operator : CG\JU
Sample : P1147-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-D

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137084.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	497	498	505	rVB	14620	16117	1.65%	0.217%
2	5.428	565	568	586	rBV	909678	901828	92.49%	12.153%
3	6.034	667	671	677	rBV4	13978	20638	2.12%	0.278%
4	6.310	715	718	721	rBV	29941	26942	2.76%	0.363%
5	6.434	735	739	749	rBV	944542	868962	89.12%	11.710%
6	6.522	749	754	758	rVB4	7677	16200	1.66%	0.218%
7	6.610	766	769	772	rBV3	20820	22249	2.28%	0.300%
8	6.781	795	798	802	rVB	362237	295384	30.29%	3.981%
9	6.922	819	822	826	rBV2	14500	16512	1.69%	0.223%
10	7.045	841	843	847	rVB3	15758	17453	1.79%	0.235%
11	7.169	860	864	867	rVB2	12283	12252	1.26%	0.165%
12	7.310	882	888	890	rBV4	10099	12211	1.25%	0.165%
13	7.345	890	894	897	rVV	673018	556333	57.06%	7.497%
14	7.369	897	898	902	rVV	21199	15445	1.58%	0.208%
15	7.422	902	907	910	rVB5	8323	11504	1.18%	0.155%
16	8.057	1012	1015	1021	rVB	441577	356810	36.59%	4.808%
17	9.133	1194	1198	1208	rBV	1118557	975080	100.00%	13.140%
18	9.216	1208	1212	1216	rVB	15574	17633	1.81%	0.238%
19	9.816	1311	1314	1324	rVB	438805	343628	35.24%	4.631%
20	10.610	1446	1449	1459	rBV	486152	456257	46.79%	6.149%
21	10.721	1465	1468	1472	rVB3	8181	12285	1.26%	0.166%
22	11.310	1564	1568	1577	rBV	359105	300325	30.80%	4.047%
23	11.839	1653	1658	1674	rBV	151590	202761	20.79%	2.732%
24	12.486	1762	1768	1774	rVB2	13507	29054	2.98%	0.392%
25	12.551	1774	1779	1784	rBV8	8181	18613	1.91%	0.251%
26	12.627	1789	1792	1801	rBV	73135	97832	10.03%	1.318%
27	12.904	1835	1839	1842	rBV	868074	704812	72.28%	9.498%
28	13.227	1887	1894	1897	rBV3	18677	31037	3.18%	0.418%
29	13.474	1933	1936	1939	rBV2	14911	14500	1.49%	0.195%
30	13.815	1989	1994	1998	rBV2	37030	58601	6.01%	0.790%
31	13.862	1998	2002	2006	rVV6	11604	25095	2.57%	0.338%
32	13.968	2017	2020	2027	rBV	299852	296414	30.40%	3.994%
33	14.062	2033	2036	2041	rVB2	11722	15233	1.56%	0.205%
34	14.127	2044	2047	2049	rBV	20057	16903	1.73%	0.228%
35	14.309	2074	2078	2082	rBV2	26263	40637	4.17%	0.548%
36	14.433	2096	2099	2102	rBV	25942	23438	2.40%	0.316%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137084.D
Acq On : 16 Jan 2024 17:39
Operator : CG\JU
Sample : P1147-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-D

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.745	2149	2152	2153	rBV	21154	18975	1.95%	0.256%
38	14.815	2161	2164	2169	rVB	59139	54863	5.63%	0.739%
39	15.086	2207	2210	2214	rVB2	19800	22828	2.34%	0.308%
40	15.245	2234	2237	2241	rBV4	13128	21794	2.24%	0.294%
41	15.462	2269	2274	2281	rBV	286079	384694	39.45%	5.184%
42	15.921	2350	2352	2357	rVB3	22158	26488	2.72%	0.357%
43	16.445	2438	2441	2453	rVB3	18609	43946	4.51%	0.592%

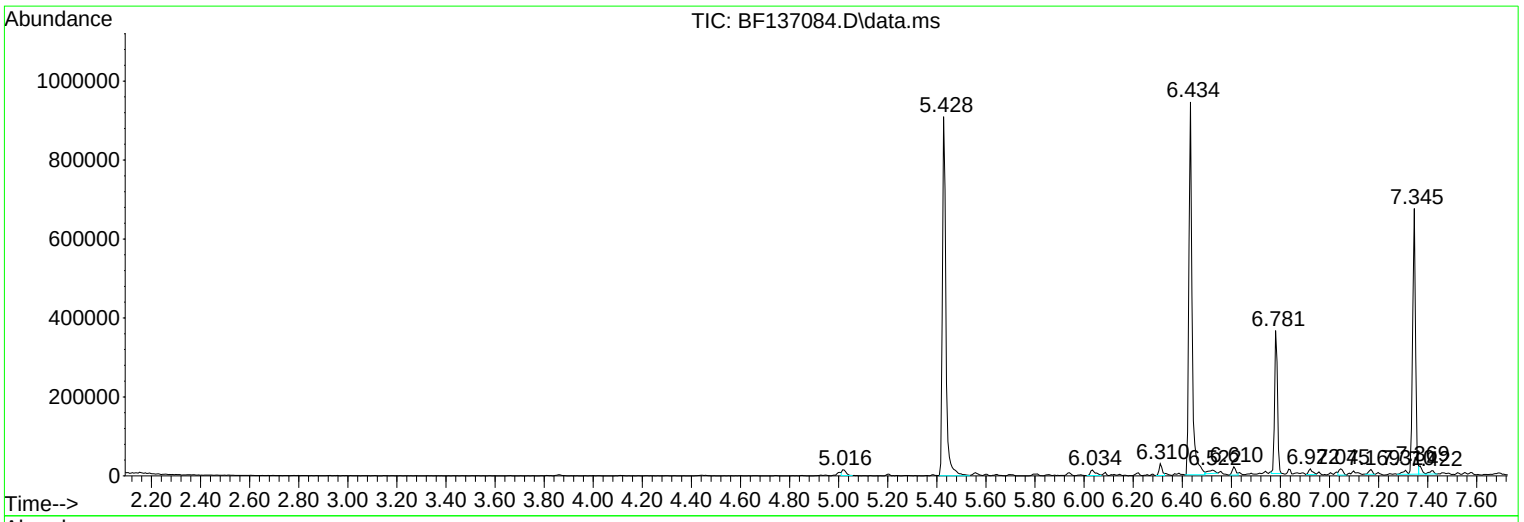
Sum of corrected areas: 7420566

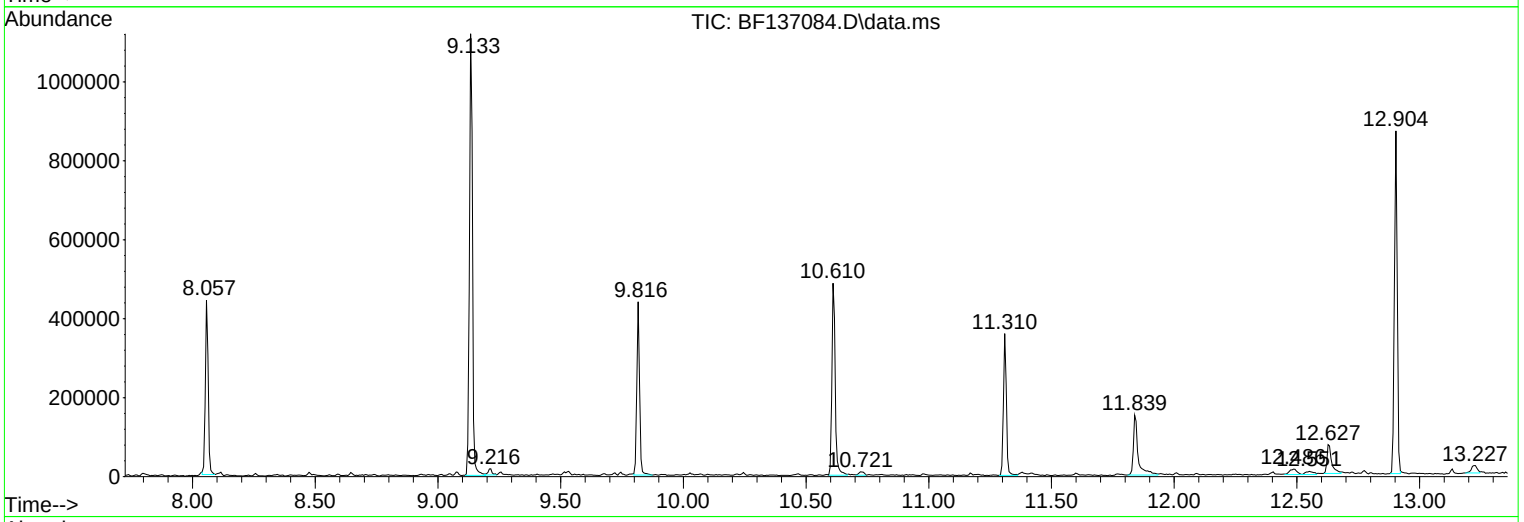
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137084.D
Acq On : 16 Jan 2024 17:39
Operator : CG\JU
Sample : P1147-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

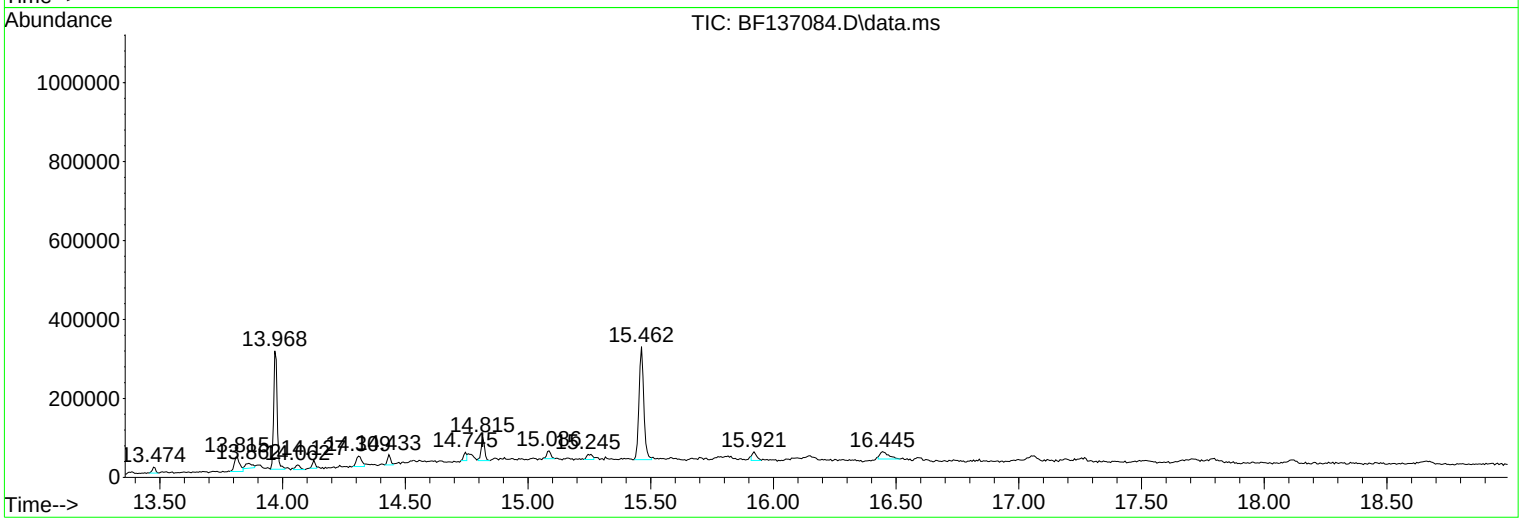
Instrument :
BNA_F
ClientSampleId :
MH-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF011624\
Data File : BF137084.D
Acq On : 16 Jan 2024 17:39
Operator : CG\JU
Sample : P1147-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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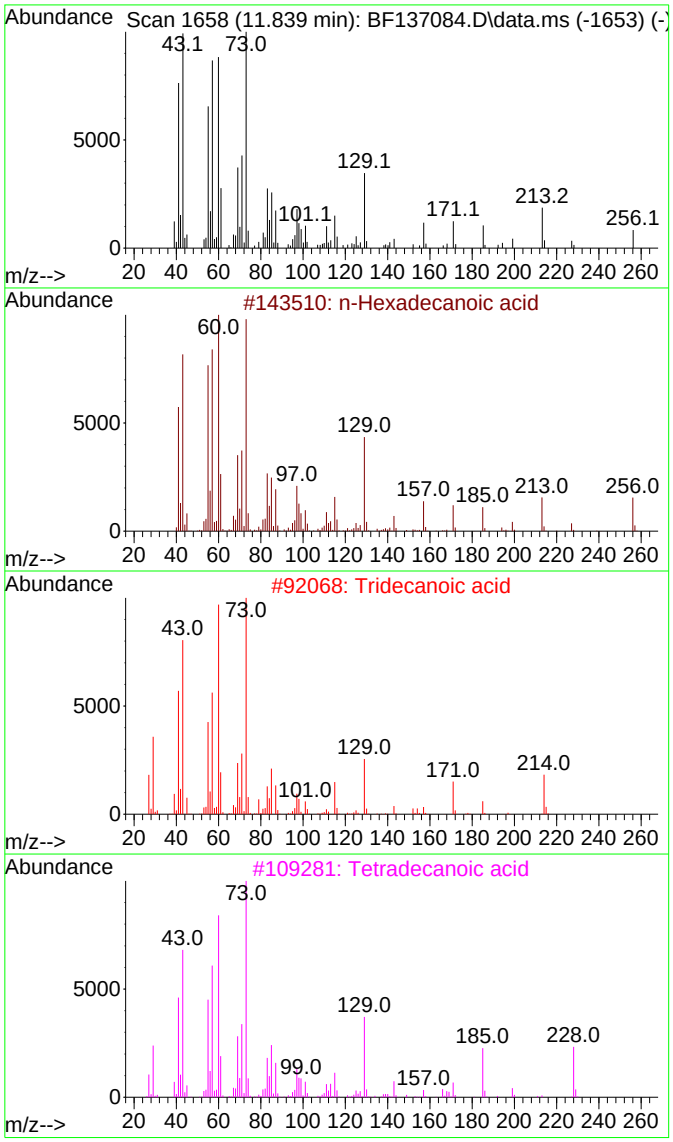
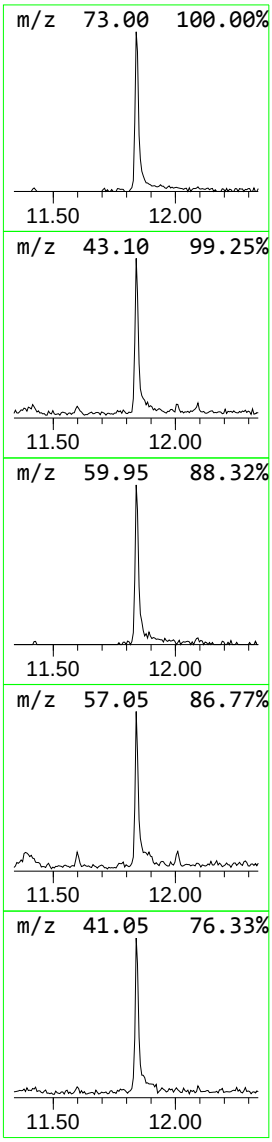
Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	13.50 ng	202761	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	Nonanoic acid	158	C9H18O2	000112-05-0	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137084.D
Acq On : 16 Jan 2024 17:39
Operator : CG\JU
Sample : P1147-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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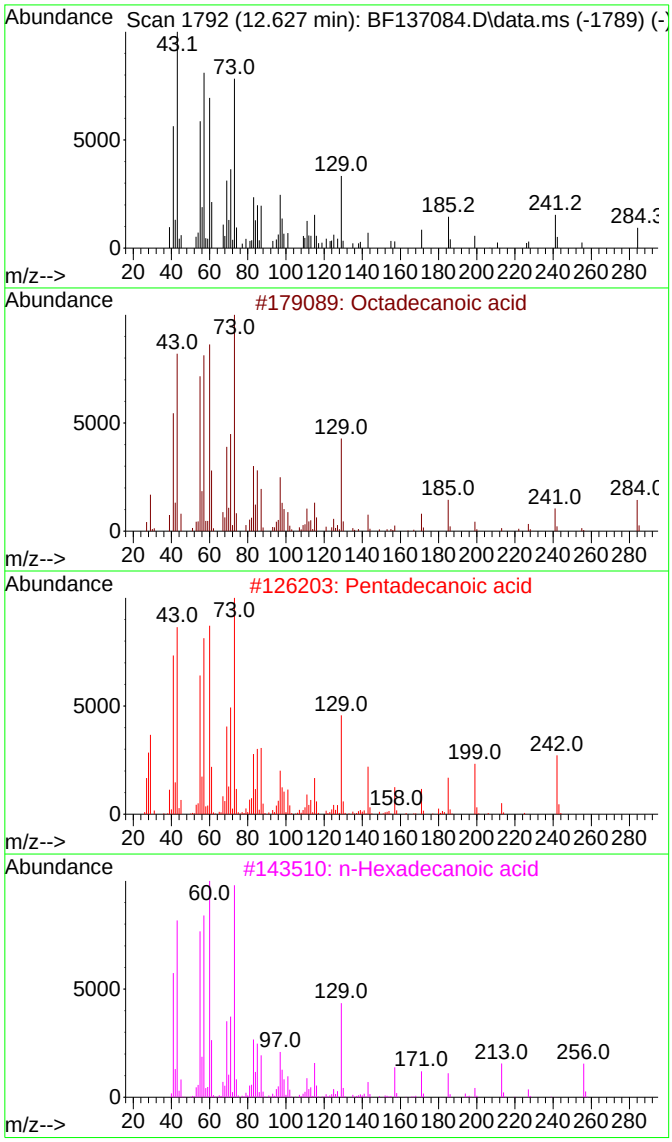
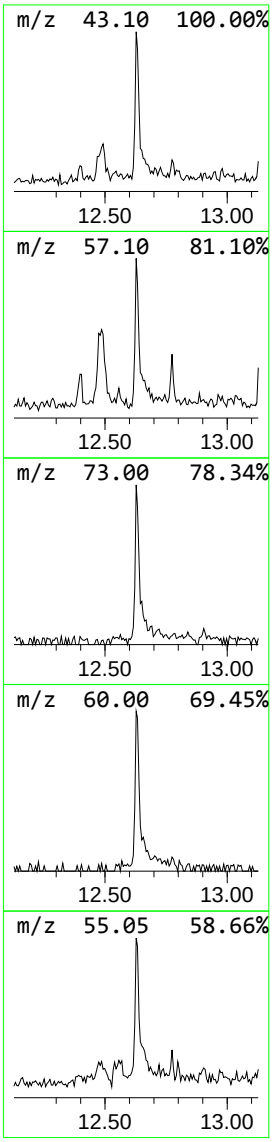
Peak Number 2 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	6.52 ng	97832	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137084.D
Acq On : 16 Jan 2024 17:39
Operator : CG\JU
Sample : P1147-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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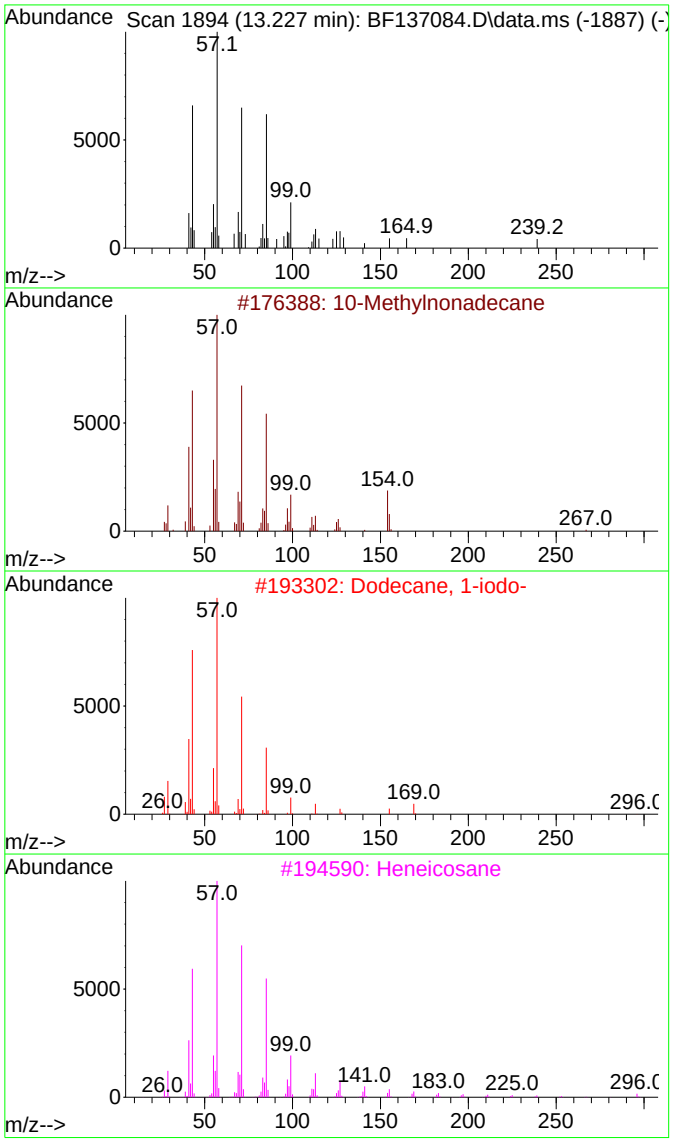
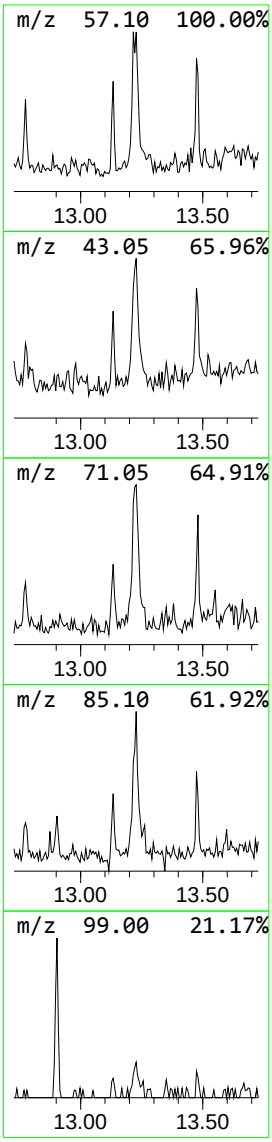
Peak Number 3 10-Methylnonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.227	2.09 ng	31037	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	72
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64
3	Heneicosane	296	C21H44	000629-94-7	64
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137084.D
Acq On : 16 Jan 2024 17:39
Operator : CG\JU
Sample : P1147-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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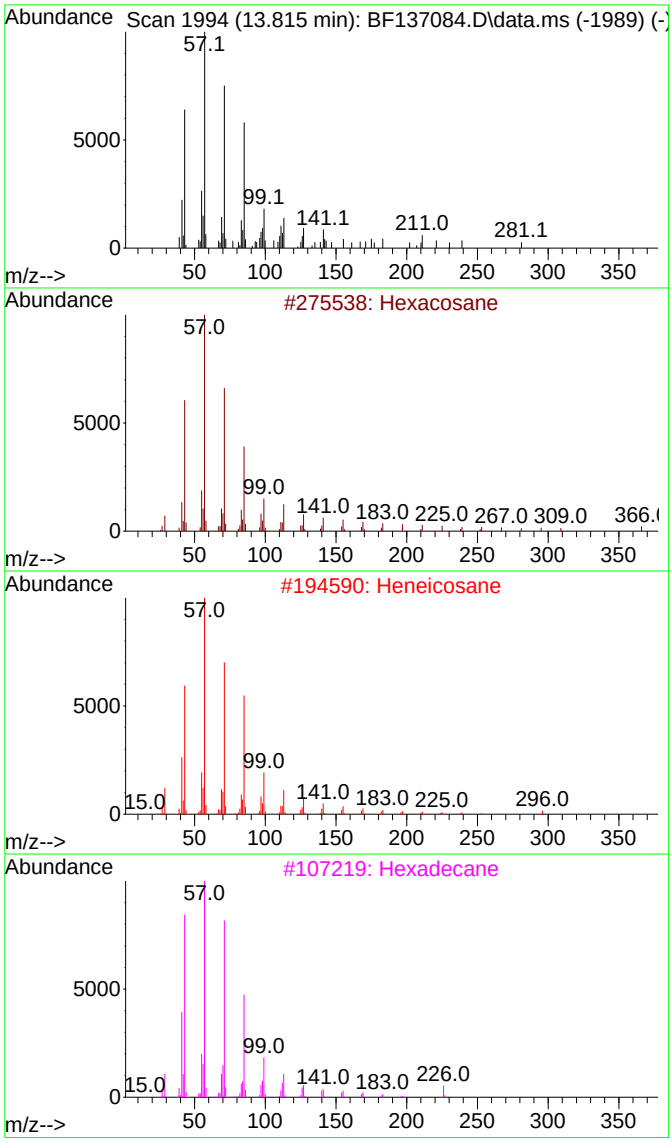
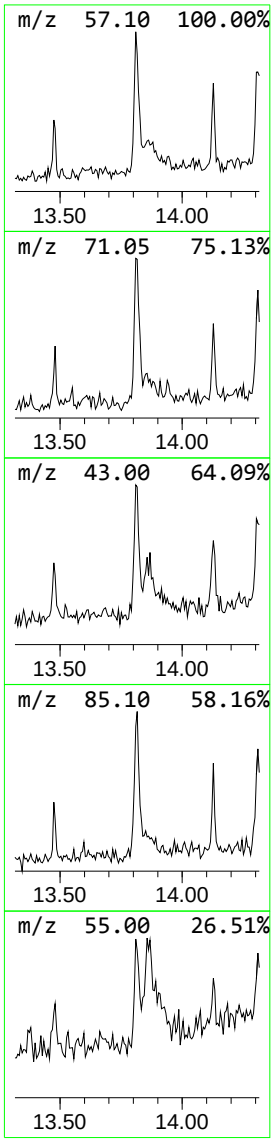
Peak Number 4 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	3.95 ng	58601	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexadecane	226	C16H34	000544-76-3	87
4	Pentacosane	352	C25H52	000629-99-2	87
5	Heptadecane	240	C17H36	000629-78-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137084.D
Acq On : 16 Jan 2024 17:39
Operator : CG\JU
Sample : P1147-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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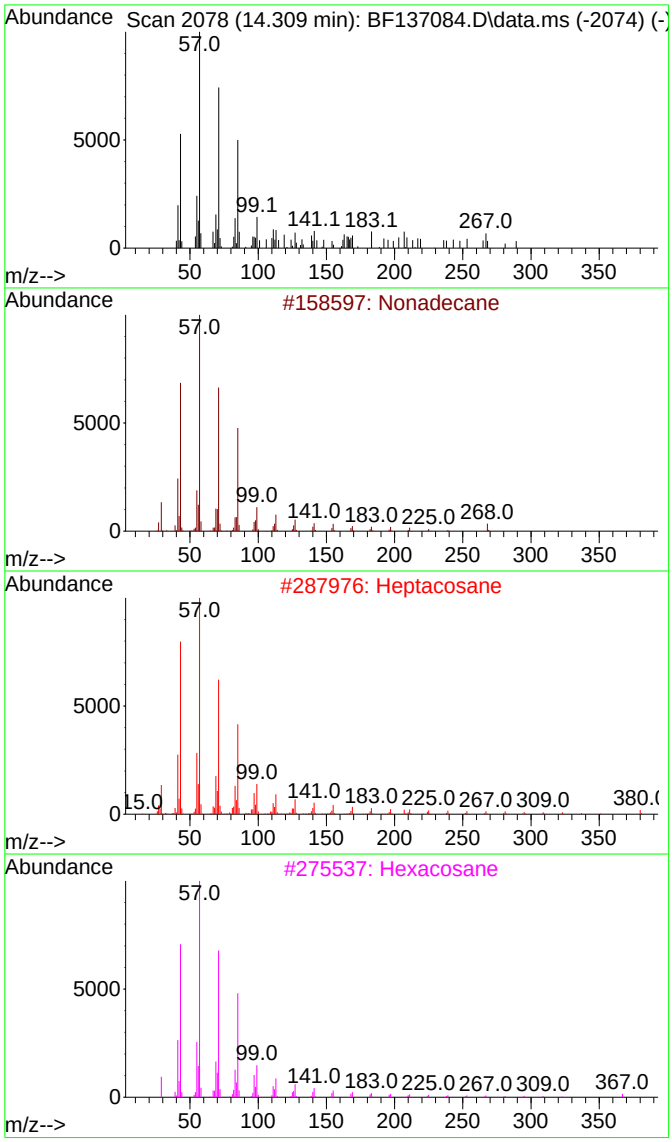
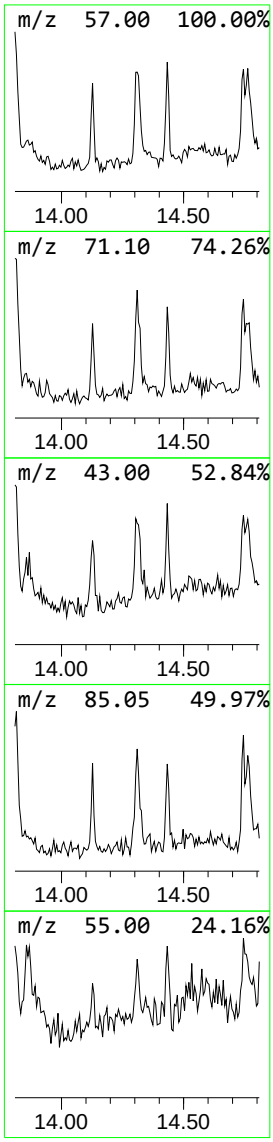
Peak Number 5 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.310	2.74 ng	40637	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heptacosane	380	C27H56	000593-49-7	83
3	Hexacosane	366	C26H54	000630-01-3	80
4	Octadecane	254	C18H38	000593-45-3	80
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137084.D
Acq On : 16 Jan 2024 17:39
Operator : CG\JU
Sample : P1147-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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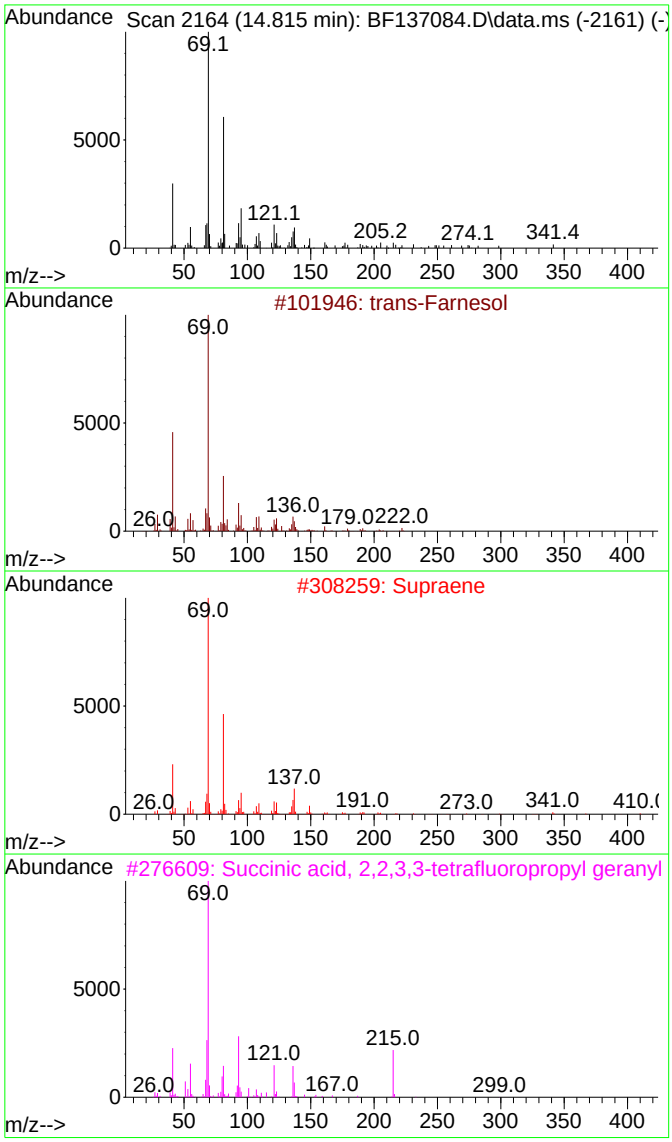
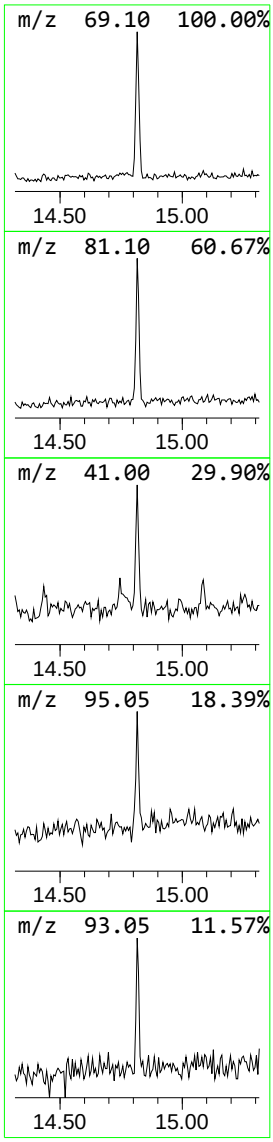
Peak Number 6 trans-Farnesol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	2.85 ng	54863	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Farnesol	222	C15H26O	000106-28-5	76
2	Supraene	410	C30H50	007683-64-9	74
3	Succinic acid, 2,2,3,3-tetrafluo...	368	C17H24F4O4	1000391-20-8	64
4	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64
5	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137084.D
Acq On : 16 Jan 2024 17:39
Operator : CG\JU
Sample : P1147-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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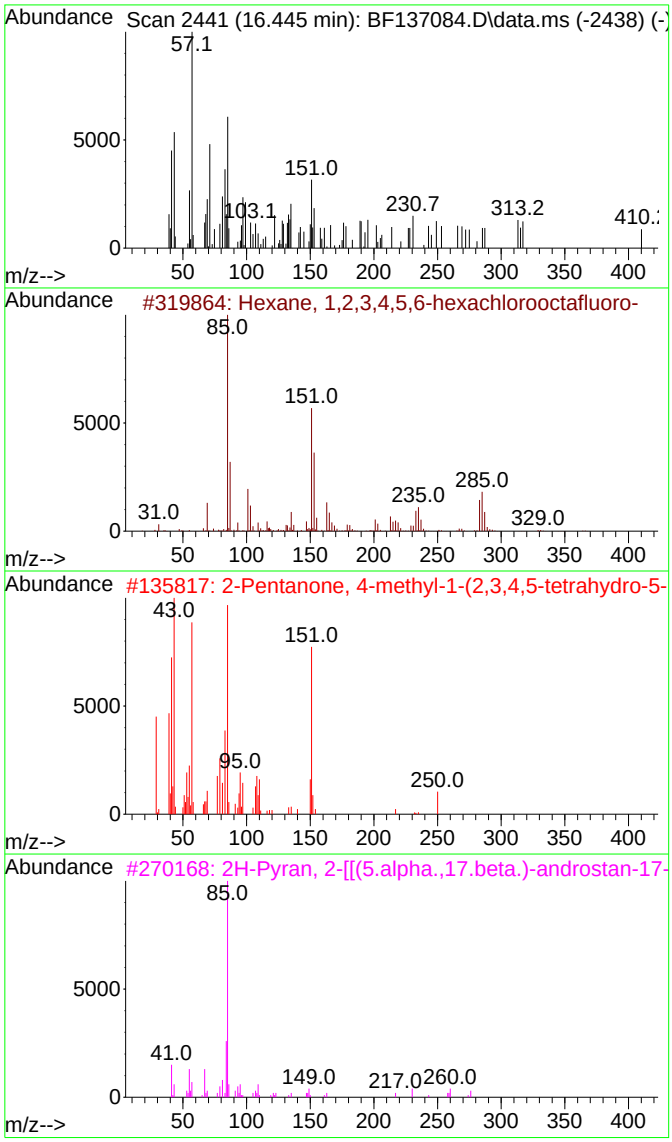
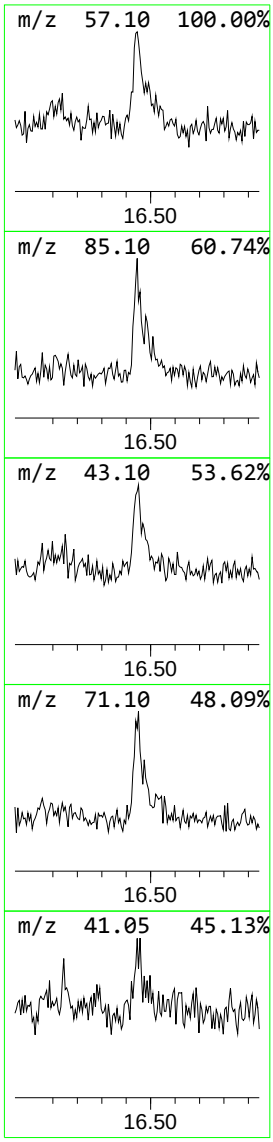
Peak Number 7 unknown16.445 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	2.28 ng	43946	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 1,2,3,4,5,6-hexachlorooc...	434	C6Cl6F8	000307-25-5	35
2	2-Pentanone, 4-methyl-1-(2,3,4,5...	250	C15H22O3	020007-82-3	16
3	2H-Pyran, 2-[[(5.alpha.,17.beta....	360	C24H40O2	055162-81-7	14
4	Ethyl 3,4-difluorocyclopentaneca...	178	C8H12F2O2	1000461-13-7	14
5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	12





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137084.D
Acq On : 16 Jan 2024 17:39
Operator : CG\JU
Sample : P1147-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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 ...	11.839	13.5	ng	202761	4	11.310	300325	20.0
Octadecanoic acid	12.627	6.5	ng	97832	4	11.310	300325	20.0
10-Methylnonade...	13.227	2.1	ng	31037	5	13.968	296414	20.0
Hexacosane	13.815	4.0	ng	58601	5	13.968	296414	20.0
Nonadecane	14.310	2.7	ng	40637	5	13.968	296414	20.0
trans-Farnesol	14.815	2.9	ng	54863	6	15.462	384694	20.0
unknown16.445	16.445	2.3	ng	43946	6	15.462	384694	20.0