LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136690.D
Acq On : 22 Dec 2023 17:37
Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

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: BF136690.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	494	498	505	rVB	62491	72766	4.99%	0.637%
2	5.428	563	568	571	rBV	1372983	1241717	85.10%	10.872%
3	6.428	734	738	741	rBV	1418807	1234818	84.63%	10.812%
4	6.781	794	798	801	rBV	565266	423756	29.04%	3.710%
5	7.340	888	893	896	rBV	882990	816463	55.96%	7.149%
6	8.057	1011	1015	1018	rBV	699831	543201	37.23%	4.756%
7	8.392	1067	1072	1079	rBV3	8896	20538	1.41%	0.180%
8	9.134	1194	1198	1201	rBV	1736970	1459088	100.00%	12.776%
9	9.810	1310	1313	1317	rBV	604637	547265	37.51%	4.792%
10	10.022	1344	1349	1355	rBV2	12892	19616	1.34%	0.172%
11	10.604	1444	1448	1458	rBV	771686	689990	47.29%	6.042%
12	10.939	1497	1505	1506	rBV5	9750	22168	1.52%	0.194%
13	10.969	1507	1510	1520	rVB5	15978	28480	1.95%	0.249%
14	11.304	1563	1567	1569	rBV	622848	496324	34.02%	4.346%
15	11.328	1569	1571	1574	rVV	107127	79746	5.47%	0.698%
16	11.375	1574	1579	1583	rVB2	20322	19442	1.33%	0.170%
17	11.839	1654	1658	1668	rVB	251791	252903	17.33%	2.214%
18	11.916	1668	1671	1674	rBV	22080	20618	1.41%	0.181%
19	12.133	1705	1708	1712	rVB4	16801	18593	1.27%	0.163%
20	12.522	1770	1774	1777	rBV	228566	203553	13.95%	1.782%
21	12.627	1787	1792	1799	rBV2	103776	125977	8.63%	1.103%
22	12.751	1808	1813	1816	rBV	177583	164748	11.29%	1.443%
23	12.898	1834	1838	1841	rVB	1226059	1017114	69.71%	8.906%
24	12.974	1846	1851	1854	rVB2	11728	16517	1.13%	0.145%
25	13.080	1867	1869	1873	rVB	25644	21575	1.48%	0.189%
26	13.186	1884	1887	1889	rBV2	18542	19185	1.31%	0.168%
27	13.704	1970	1975	1978	rBV2	23477	29877	2.05%	0.262%
28	13.804	1989	1992	1997	rVB3	17593	20846	1.43%	0.183%
29	13.874	2000	2004	2012	rVV6	27510	67005	4.59%	0.587%
30	13.957	2012	2018	2021	rVV2	468713	515760	35.35%	4.516%
31	13.980	2021	2022	2028	rVB	101024	73335	5.03%	0.642%
32	14.345	2081	2084	2087	rVB2	19500	18599	1.27%	0.163%
33	14.392	2087	2092	2095	rBV6	23311	42549	2.92%	0.373%
34	14.433	2096	2099	2103	rVB3	34483	40317	2.76%	0.353%
35	14.592	2123	2126	2131	rBV	69622	65222	4.47%	0.571%
36	14.816	2160	2164	2171	rVB4	44628	58319	4.00%	0.511%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136690.D
Acq On : 22 Dec 2023 17:37
Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

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	14.998	2191	2195	2198	rBV	90981	122078	8.37%	1.069%
38	15.086	2206	2210	2212	rBV4	14662	18042	1.24%	0.158%
39	15.251	2234	2238	2243	rVB3	36976	53255	3.65%	0.466%
40	15.304	2243	2247	2253	rVB2	54869	68445	4.69%	0.599%
41	15.368	2254	2258	2263	rVB	73144	88424	6.06%	0.774%
42	15.433	2264	2269	2273	rBV	344555	411098	28.17%	3.600%
43	15.751	2319	2323	2328	rVB3	30444	45694	3.13%	0.400%
44	16.363	2422	2427	2432	rVB5	21442	45105	3.09%	0.395%
45	16.921	2516	2522	2529	rVB3	27997	60679	4.16%	0.531%

Sum of corrected areas: 11420810

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
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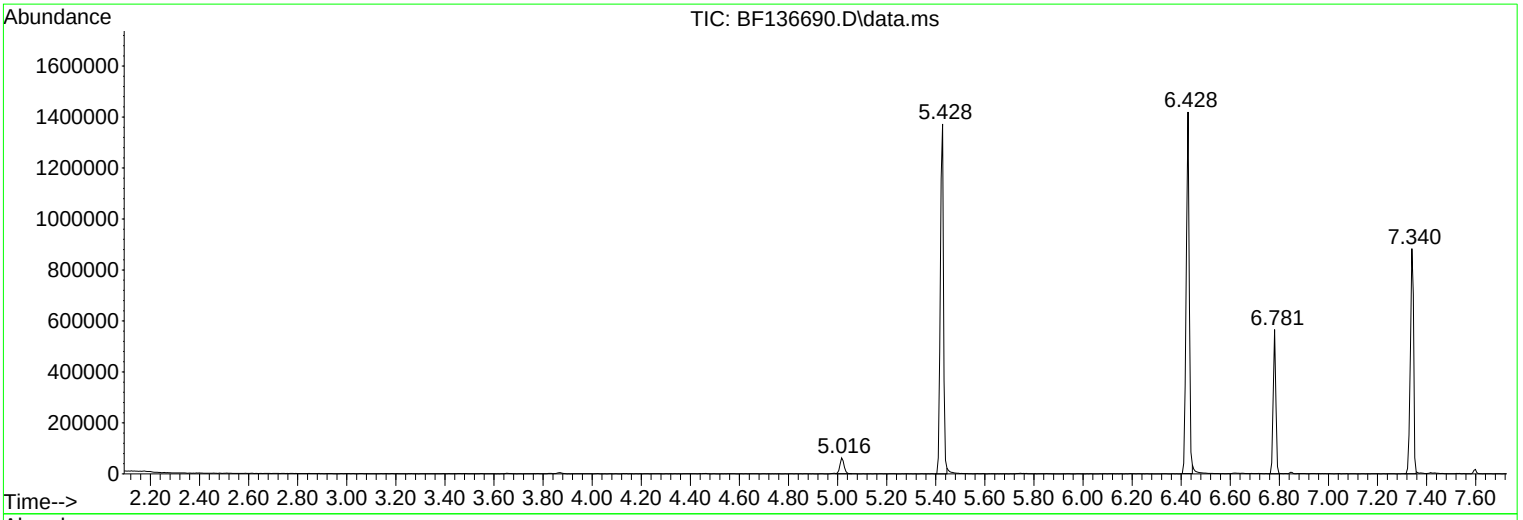
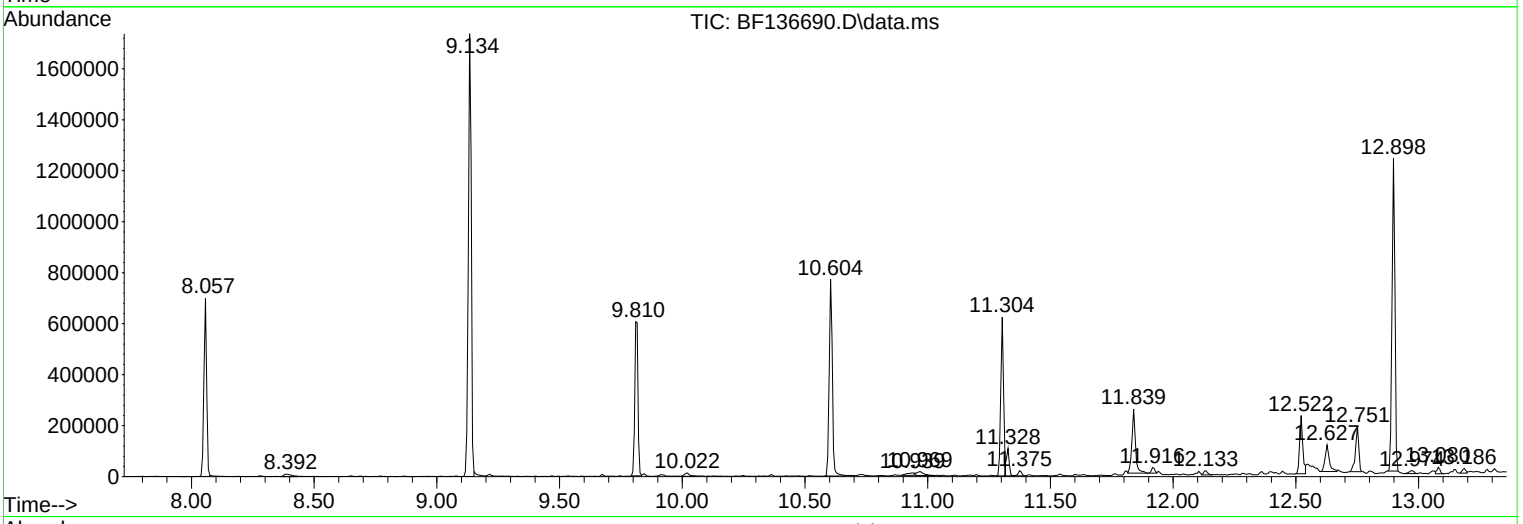
Misc :
ALS Vial : 4 Sample Multiplier: 1

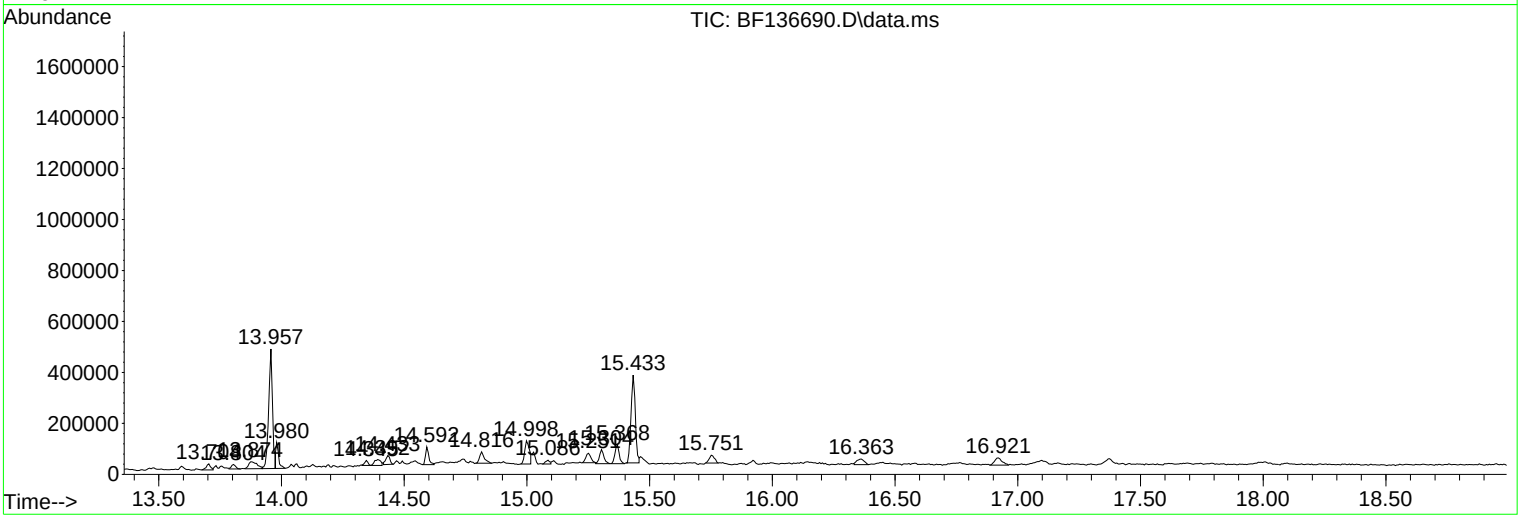
Instrument :
BNA_F
ClientSampleId :
72-12000

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\BF122223\
Data File : BF136690.D
Acq On : 22 Dec 2023 17:37
Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

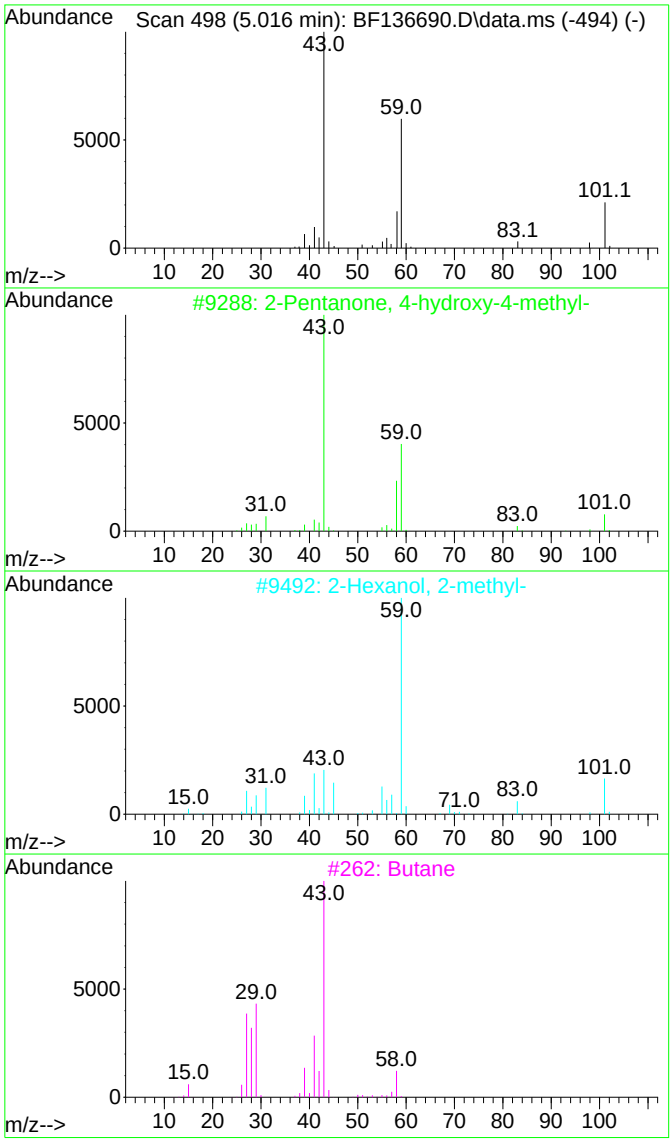
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

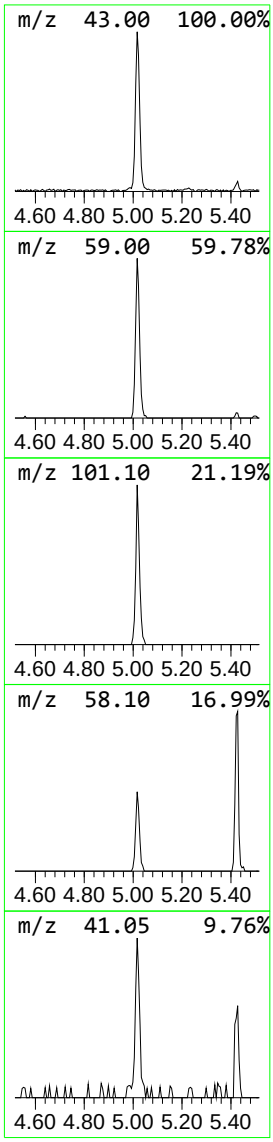
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	3.43 ng	72766	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3	Butane	58	C4H10	000106-97-8	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136690.D
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Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

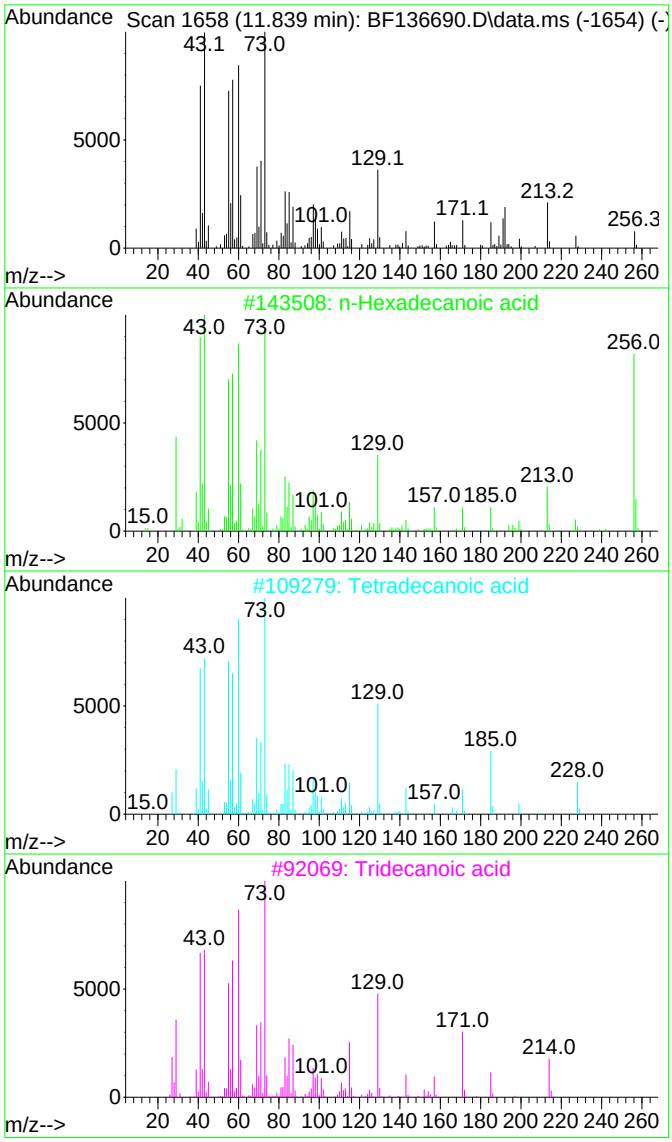
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

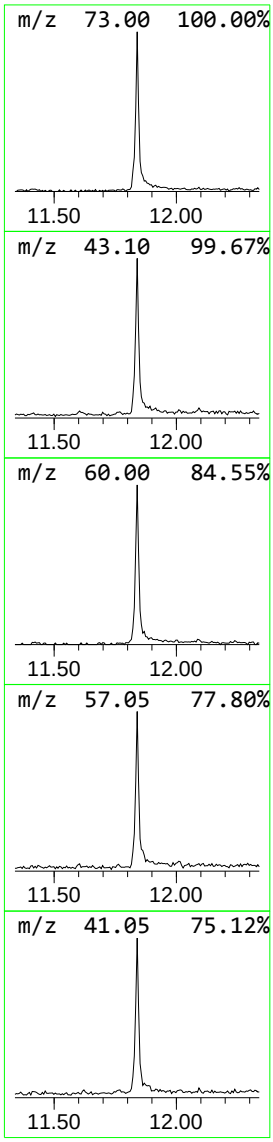
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	10.19 ng	252903	Phenanthrene-d10	11.304

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	Tridecanoic acid	214	C13H26O2	000638-53-9	96
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136690.D
Acq On : 22 Dec 2023 17:37
Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

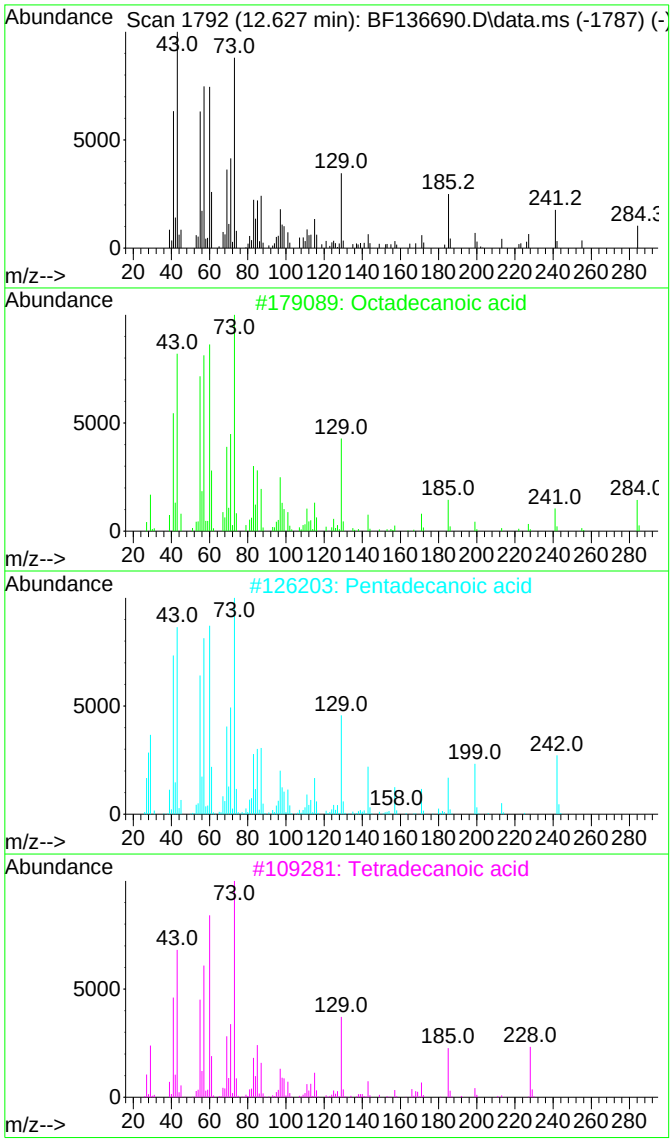
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

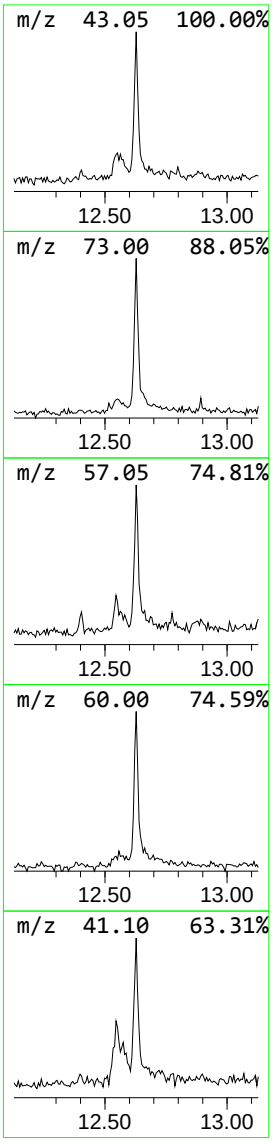
****

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.628	5.08 ng	125977	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Undecanoic acid	186	C11H22O2	000112-37-8	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136690.D
Acq On : 22 Dec 2023 17:37
Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

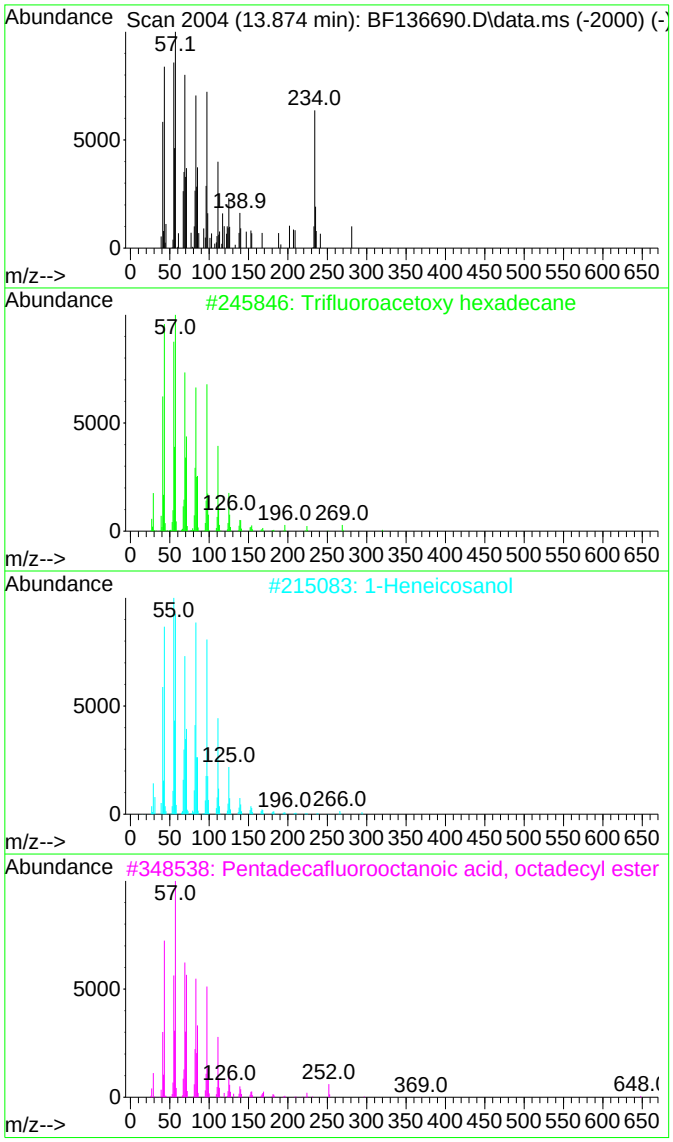
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

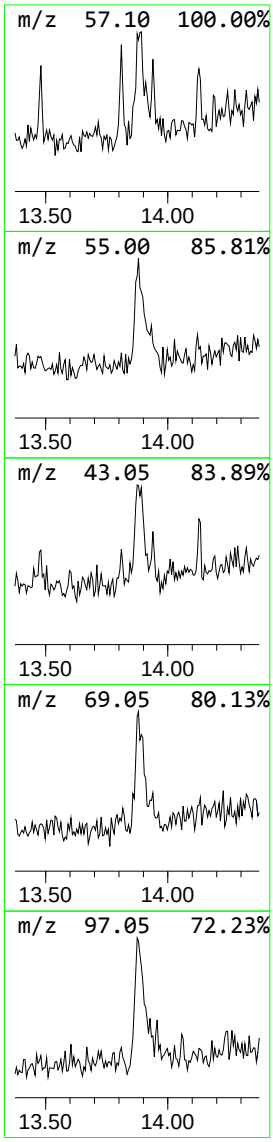
****

Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.60 ng	67005	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	64
2	1-Heneicosanol	312	C21H44O	015594-90-8	62
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	58
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	58
5	1-Octadecanol	270	C18H38O	000112-92-5	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136690.D
Acq On : 22 Dec 2023 17:37
Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

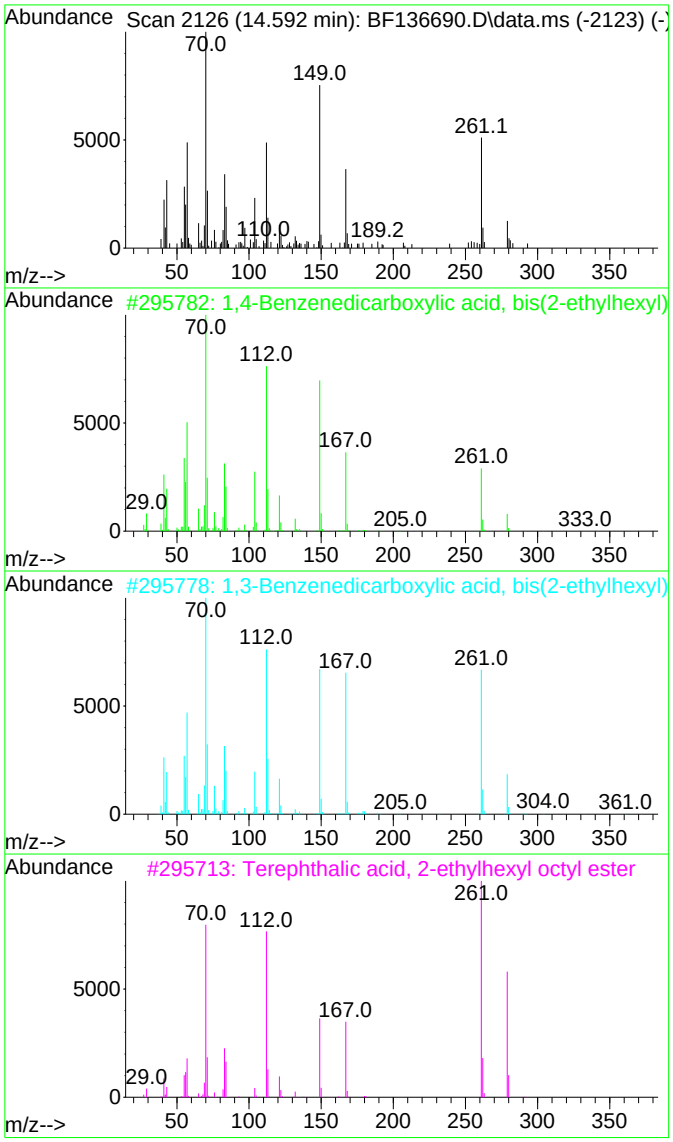
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

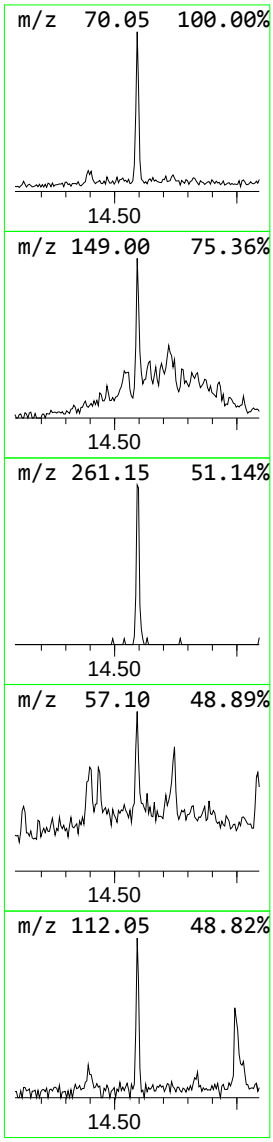
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.592	2.53 ng	65222	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	53
3	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	47
4	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	47
5	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	38





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

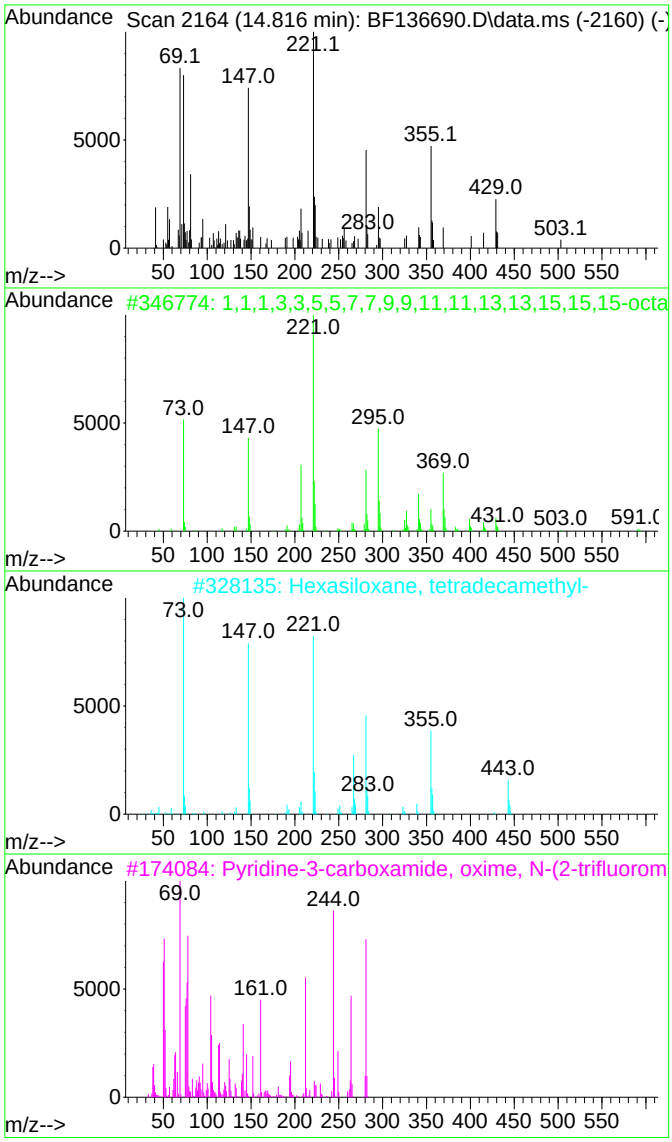
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

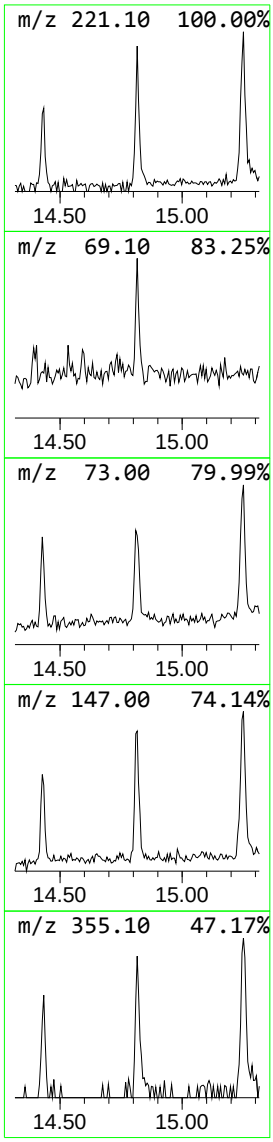
****

Peak Number 6 unknown14.816 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	2.84 ng	58319	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	37
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	32
3	Pyridine-3-carboxamide, oxime, N...	281	C13H10F3N3O	288246-53-7	18
4	Formic acid, (3,5-dinitrophenyl)...	341	C13H15N3O8	1000158-07-8	11
5	1,2,4-Benzenetricarboxylic acid,...	252	C12H12O6	002459-10-1	10





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ALS Vial : 4 Sample Multiplier: 1

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BNA_F
ClientSampleId :
72-12000

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

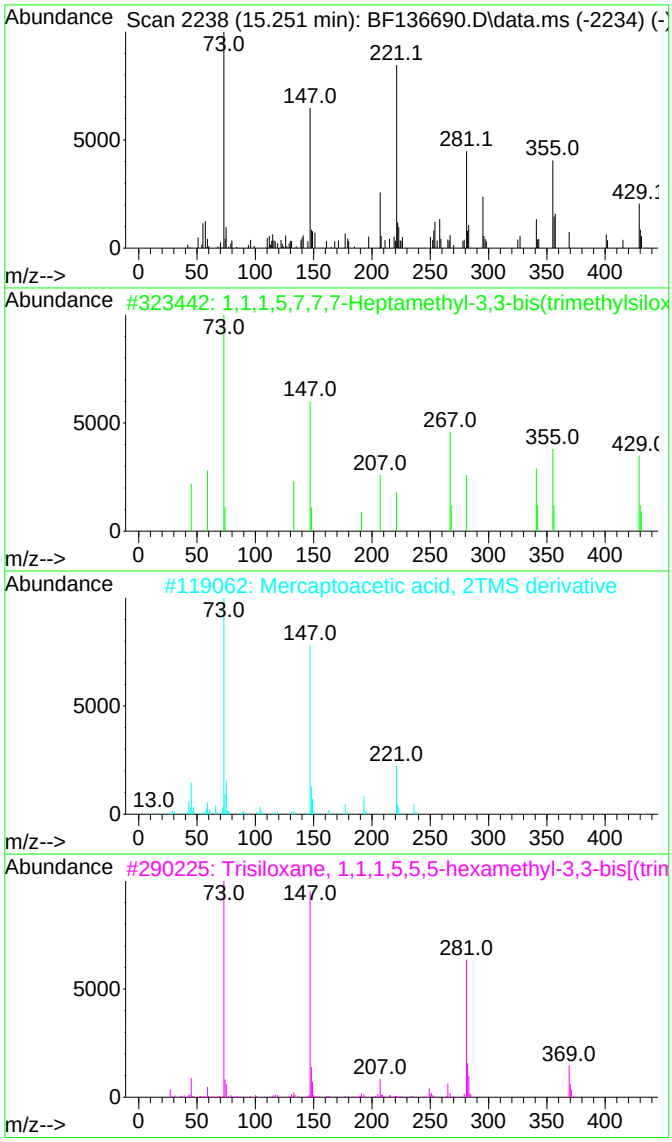
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

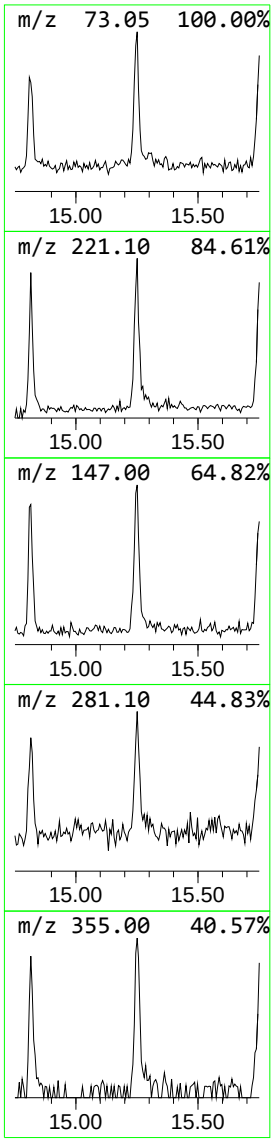
****

Peak Number 7 unknown15.251 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.251	2.59 ng	53255	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	32
2	Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	25
3	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	14
4	4H-Pyrido[1,2-a]pyrimidine-3-car...	221	C11H15N3O2	064399-29-7	14
5	1,2,4-Benzenetricarboxylic acid,...	252	C12H12O6	002459-10-1	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136690.D
Acq On : 22 Dec 2023 17:37
Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

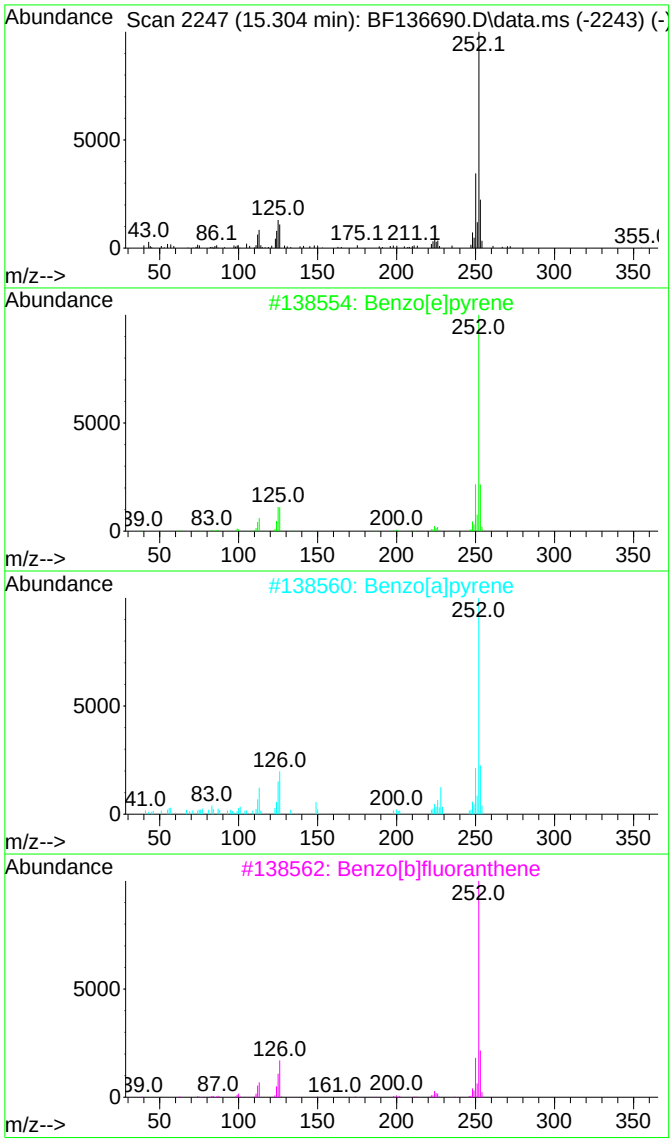
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

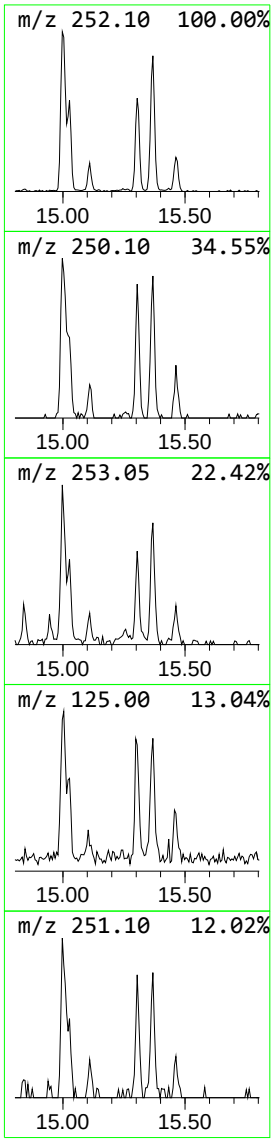
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.304	3.33 ng	68445	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	95
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Perylene	252	C20H12	000198-55-0	90





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Data File : BF136690.D
Acq On : 22 Dec 2023 17:37
Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

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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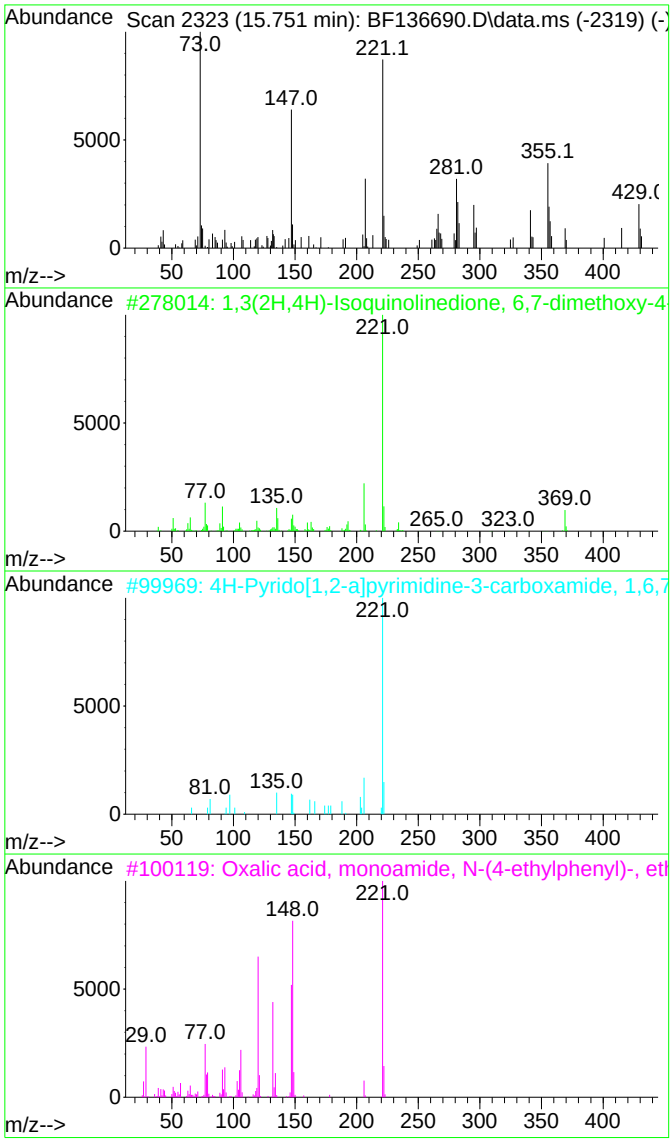
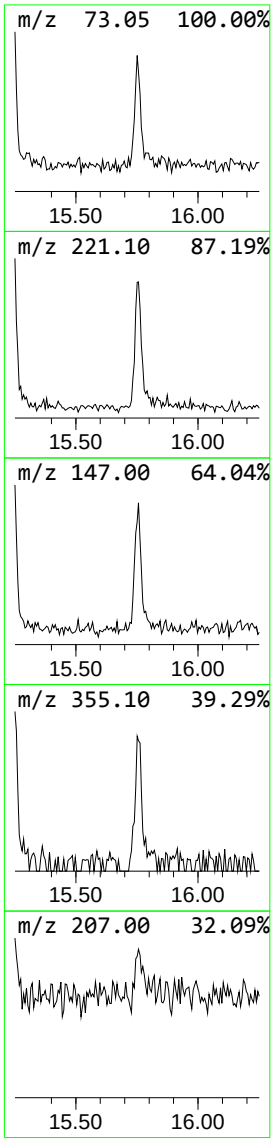
Peak Number 9 unknown15.751 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	2.22 ng	45694	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3(2H,4H)-Isoquinolinedione, 6,...	369	C20H19NO6	1000115-82-7	14
2	4H-Pyrido[1,2-a]pyrimidine-3-car...	221	C11H15N3O2	064399-29-7	14
3	Oxalic acid, monoamide, N-(4-eth...	221	C12H15NO3	1000309-57-9	12
4	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	11
5	7-Methylimidazo[1,2-a]pyrimidin-...	221	C10H15N3OSi	1010468-48-3	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136690.D
Acq On : 22 Dec 2023 17:37
Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

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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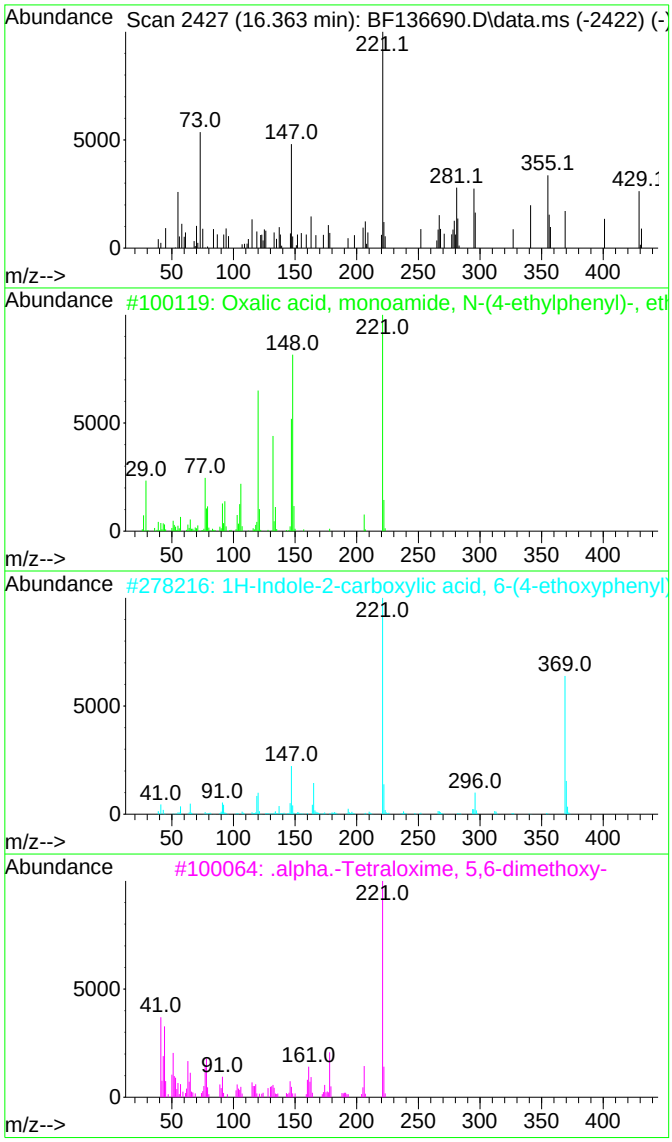
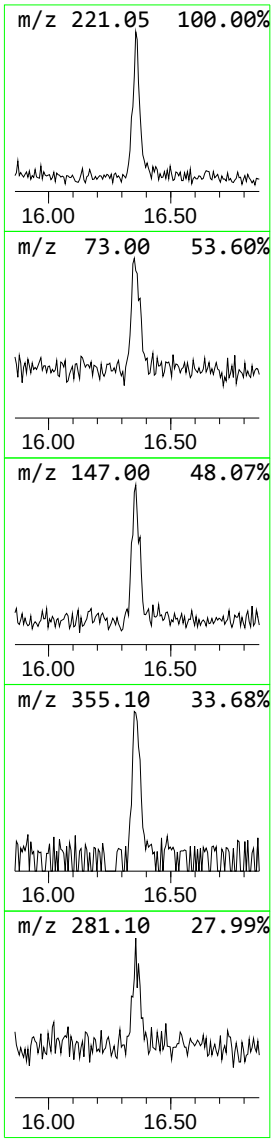
Peak Number 10 unknown16.363 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.363	2.19 ng	45105	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, monoamide, N-(4-eth...	221	C12H15NO3	1000309-57-9	35
2	1H-Indole-2-carboxylic acid, 6-(...	369	C22H27NO4	1000316-17-3	35
3	.alpha.-Tetraloxime, 5,6-dimethoxy-	221	C12H15NO3	023923-10-6	22
4	2-Hydroxy-5-morpholinomethyl-2,4...	221	C12H15NO3	1000242-00-2	18
5	1,2,4-Benzenetricarboxylic acid,...	252	C12H12O6	002459-10-1	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136690.D
Acq On : 22 Dec 2023 17:37
Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

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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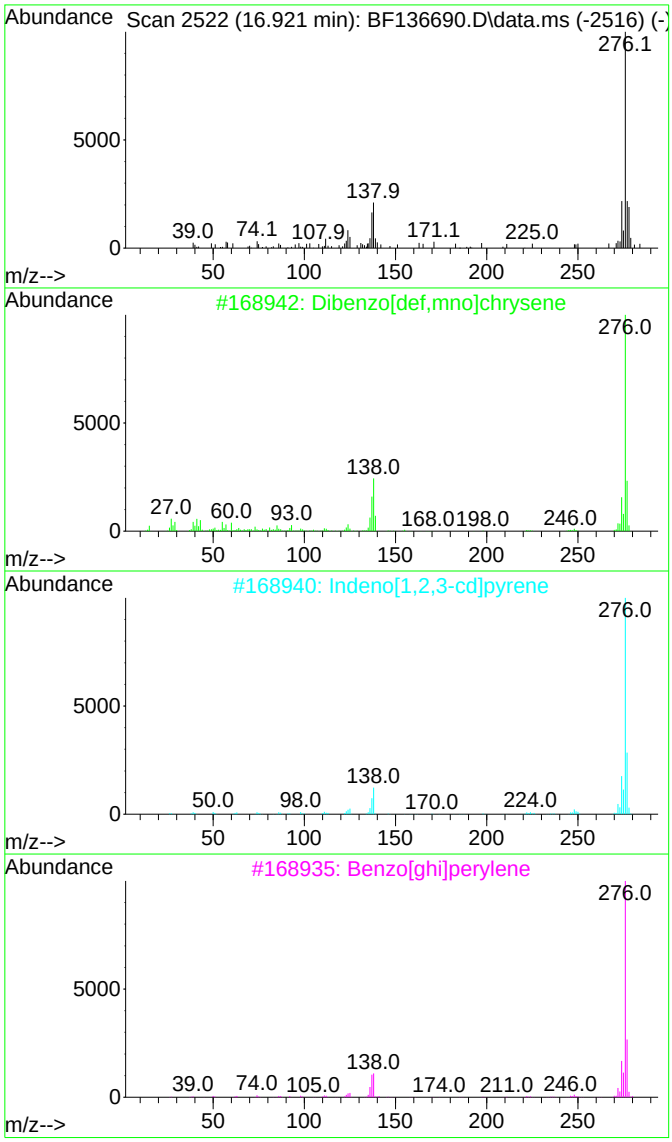
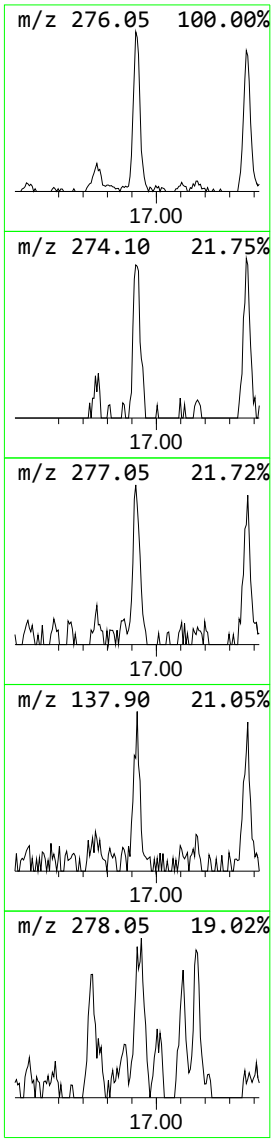
Peak Number 11 Dibenzo[def,mno]chrysene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.921	2.95 ng	60679	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	81
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	74
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	58
4	2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	50
5	1H-Pyrazole-4-sulfonamide, 2TMS	291	C9H21N3O2SSi2	1000501-56-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136690.D
Acq On : 22 Dec 2023 17:37
Operator : CG\JU
Sample : 05914-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

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
2-Pentanone, 4-...	5.016	3.4	ng	72766	1	6.781	423756	20.0
n-Hexadecanoic ...	11.839	10.2	ng	252903	4	11.304	496324	20.0
Octadecanoic acid	12.628	5.1	ng	125977	4	11.304	496324	20.0
Trifluoroacetox...	13.874	2.6	ng	67005	5	13.957	515760	20.0
1,4-Benzenedica...	14.592	2.5	ng	65222	5	13.957	515760	20.0
unknown14.816	14.816	2.8	ng	58319	6	15.433	411098	20.0
unknown15.251	15.251	2.6	ng	53255	6	15.433	411098	20.0
Benzo[e]pyrene	15.304	3.3	ng	68445	6	15.433	411098	20.0
unknown15.751	15.751	2.2	ng	45694	6	15.433	411098	20.0
unknown16.363	16.363	2.2	ng	45105	6	15.433	411098	20.0
Dibenzo[def,mno...	16.921	3.0	ng	60679	6	15.433	411098	20.0