LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133110.D
Acq On : 27 Apr 2023 20:27
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133110.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.710	271	276	282	rVB	58168	82399	2.25%	0.239%
2	4.910	474	480	485	rBV	113276	133814	3.66%	0.388%
3	5.340	549	553	559	rVB	1337214	1174563	32.14%	3.408%
4	6.175	689	695	701	rBV3	66314	78666	2.15%	0.228%
5	6.369	724	728	736	rBV	1497689	1287413	35.23%	3.735%
6	6.734	786	790	793	rBV	2904844	2316913	63.40%	6.723%
7	7.140	856	859	868	rBV4	40522	63199	1.73%	0.183%
8	7.292	879	885	888	rBV	1220415	935667	25.60%	2.715%
9	8.022	1005	1009	1011	rBV	3610119	3077579	84.21%	8.930%
10	8.039	1011	1012	1014	rVB	169811	79512	2.18%	0.231%
11	8.728	1127	1129	1134	rVB	102328	73845	2.02%	0.214%
12	8.775	1134	1137	1143	rBV	152598	143968	3.94%	0.418%
13	9.092	1187	1191	1194	rVB	2189955	1619826	44.32%	4.700%
14	9.186	1204	1207	1210	rBV2	45229	60003	1.64%	0.174%
15	9.628	1277	1282	1285	rBV	88604	89388	2.45%	0.259%
16	9.769	1300	1306	1309	rBV	3613999	3147455	86.12%	9.132%
17	9.798	1309	1311	1320	rVB2	85261	109879	3.01%	0.319%
18	9.975	1338	1341	1344	rVB2	82203	77934	2.13%	0.226%
19	10.175	1371	1375	1379	rBV5	59196	90177	2.47%	0.262%
20	10.481	1422	1427	1430	rBV	261523	271660	7.43%	0.788%
21	10.551	1436	1439	1444	rBV	762595	620699	16.98%	1.801%
22	10.680	1458	1461	1462	rBV2	103181	84994	2.33%	0.247%
23	10.904	1496	1499	1502	rBV	1065775	821987	22.49%	2.385%
24	10.975	1507	1511	1515	rBV3	86912	150679	4.12%	0.437%
25	11.051	1522	1524	1528	rBV	53866	57453	1.57%	0.167%
26	11.251	1554	1558	1560	rBV	3034630	2532495	69.30%	7.348%
27	11.275	1560	1562	1564	rVV	621764	481717	13.18%	1.398%
28	11.322	1567	1570	1574	rVB2	226479	215158	5.89%	0.624%
29	11.480	1594	1597	1600	rBV	104589	88560	2.42%	0.257%
30	11.751	1641	1643	1645	rBV	106959	86537	2.37%	0.251%
31	11.792	1646	1650	1654	rBV2	853915	850172	23.26%	2.467%
32	12.069	1694	1697	1702	rVB	343858	337290	9.23%	0.979%
33	12.463	1761	1764	1767	rBV	844650	726550	19.88%	2.108%
34	12.580	1782	1784	1788	rBV2	387899	347681	9.51%	1.009%
35	12.686	1800	1802	1805	rVB	710861	615549	16.84%	1.786%
36	12.839	1825	1828	1831	rBV	1155675	998965	27.33%	2.899%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133110.D
Acq On : 27 Apr 2023 20:27
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.892	2004	2007	2010	rBV	1715082	1666825	45.61%	4.836%
38	14.104	2040	2043	2047	rVB	2881134	2829496	77.42%	8.210%
39	14.263	2067	2070	2072	rBV	856922	704029	19.26%	2.043%
40	15.333	2249	2252	2254	rVB	823592	781842	21.39%	2.269%
41	16.333	2416	2422	2431	rVB	1930327	3654534	100.00%	10.604%
42	17.698	2650	2654	2661	rVB	444699	897347	24.55%	2.604%

Sum of corrected areas: 34464419

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
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Acq On : 27 Apr 2023 20:27
Operator : CG\JU
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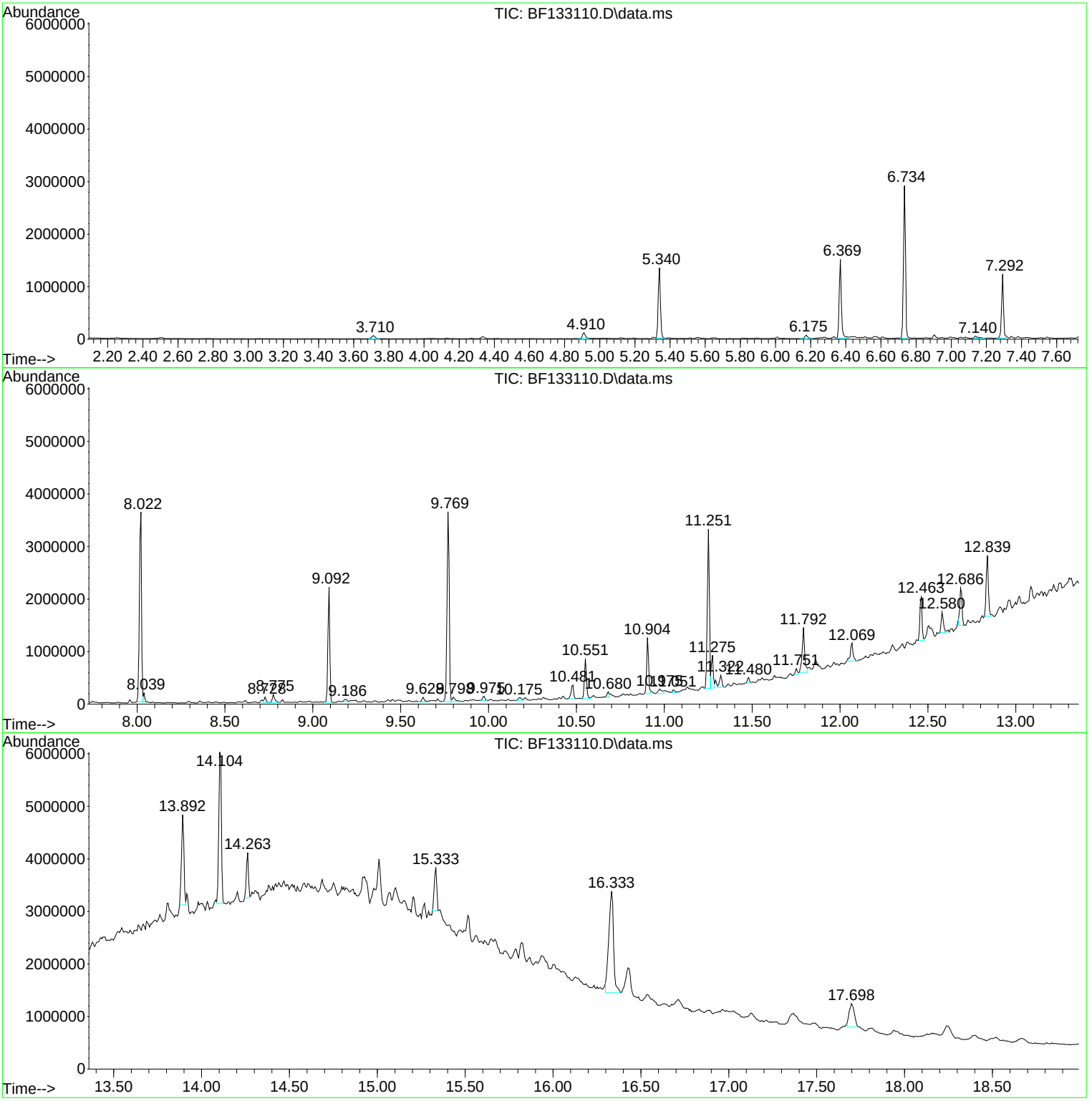
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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\BF042723\
Data File : BF133110.D
Acq On : 27 Apr 2023 20:27
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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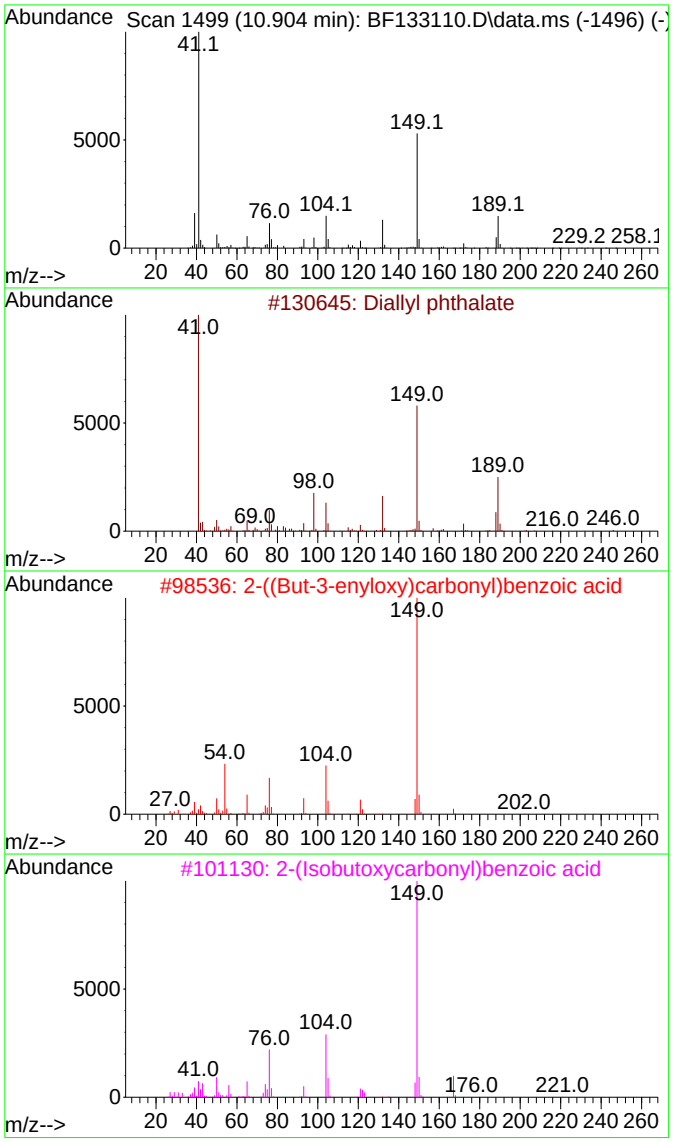
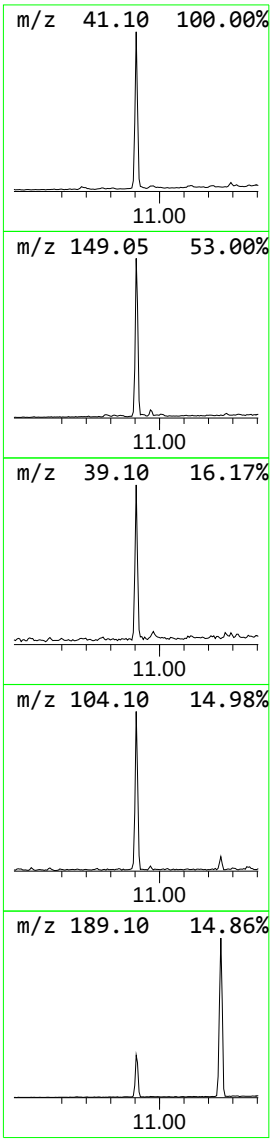
Peak Number 1 Diallyl phthalate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.904	6.49 ng	821987	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diallyl phthalate	246	C14H14O4	000131-17-9	83
2	2-((But-3-enyloxy)carbonyl)benzo...	220	C12H12O4	113793-34-3	50
3	2-(Isobutoxycarbonyl)benzoic acid	222	C12H14O4	030833-53-5	50
4	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	47
5	2-Hydroxy-1-isoindolinone	149	C8H7NO2	1000289-12-0	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133110.D
Acq On : 27 Apr 2023 20:27
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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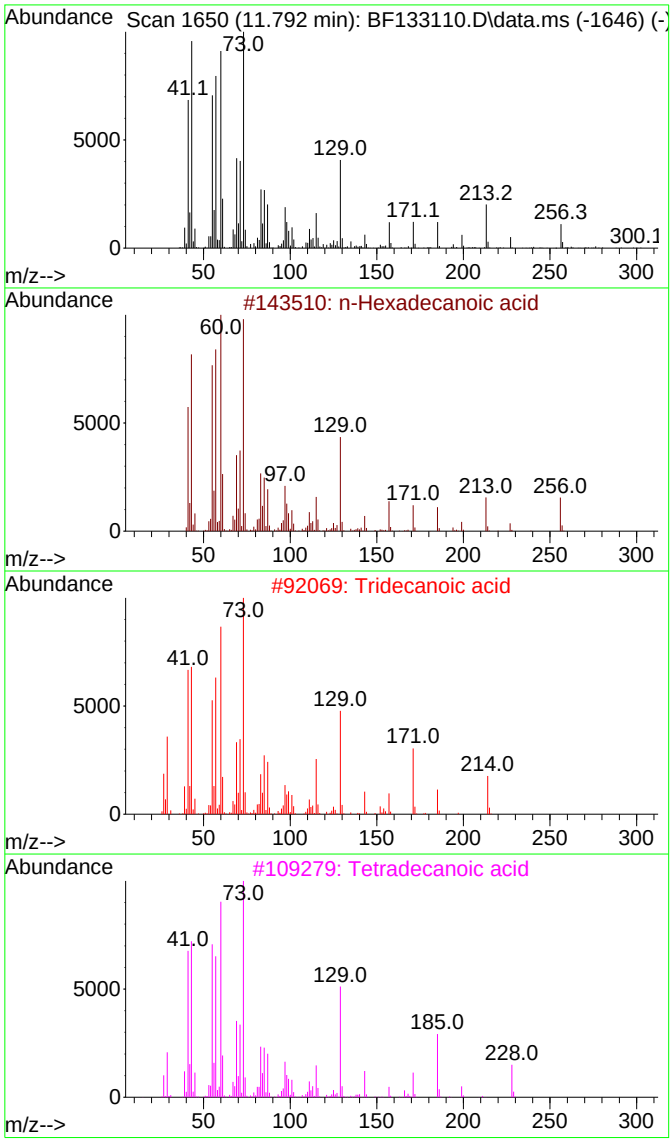
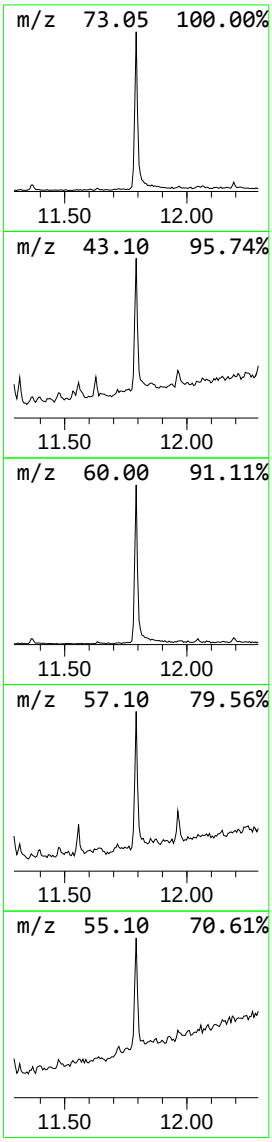
Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	6.71 ng	850172	Phenanthrene-d10	11.251

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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133110.D
Acq On : 27 Apr 2023 20:27
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

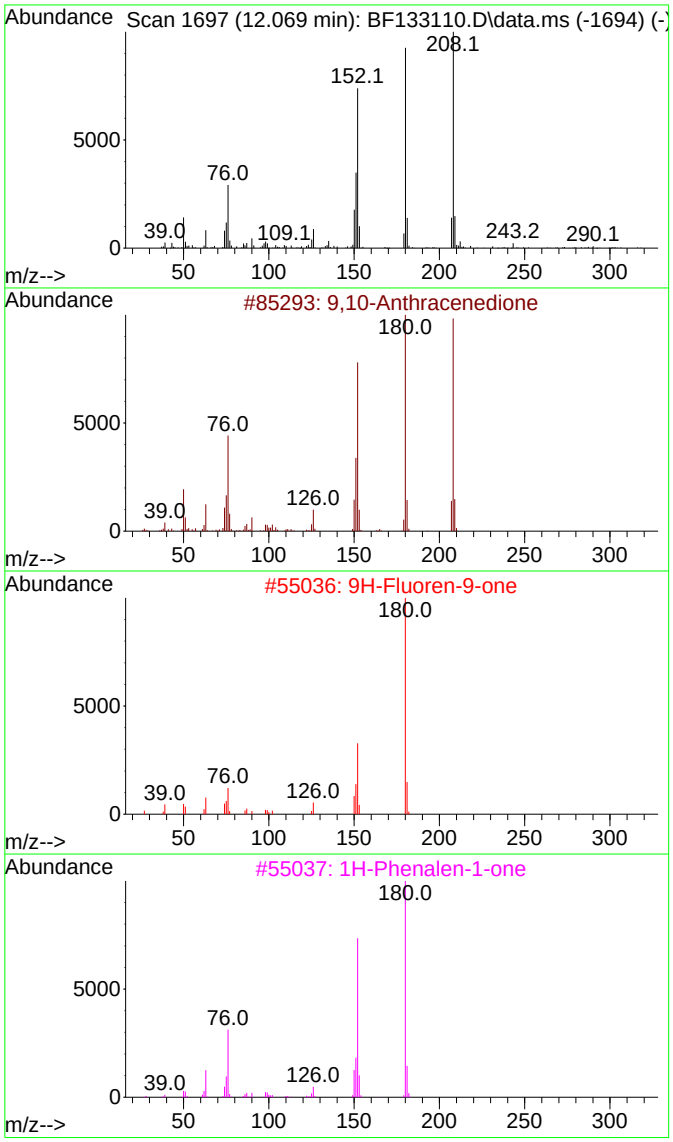
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

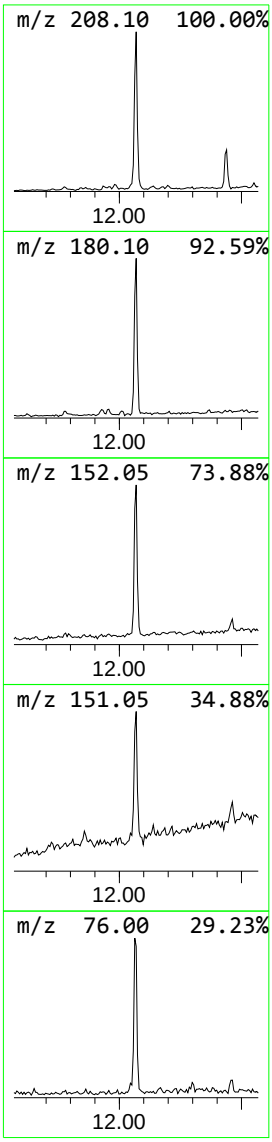
****

Peak Number 3 9,10-Anthracenedione Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.069	2.66 ng	337290	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	98
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	90
3	1H-Phenalen-1-one	180	C13H8O	000548-39-0	64
4	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	64
5	2-(Dicyanomethylene)indene-1,3-d...	208	C12H4N2O2	016954-74-8	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133110.D
Acq On : 27 Apr 2023 20:27
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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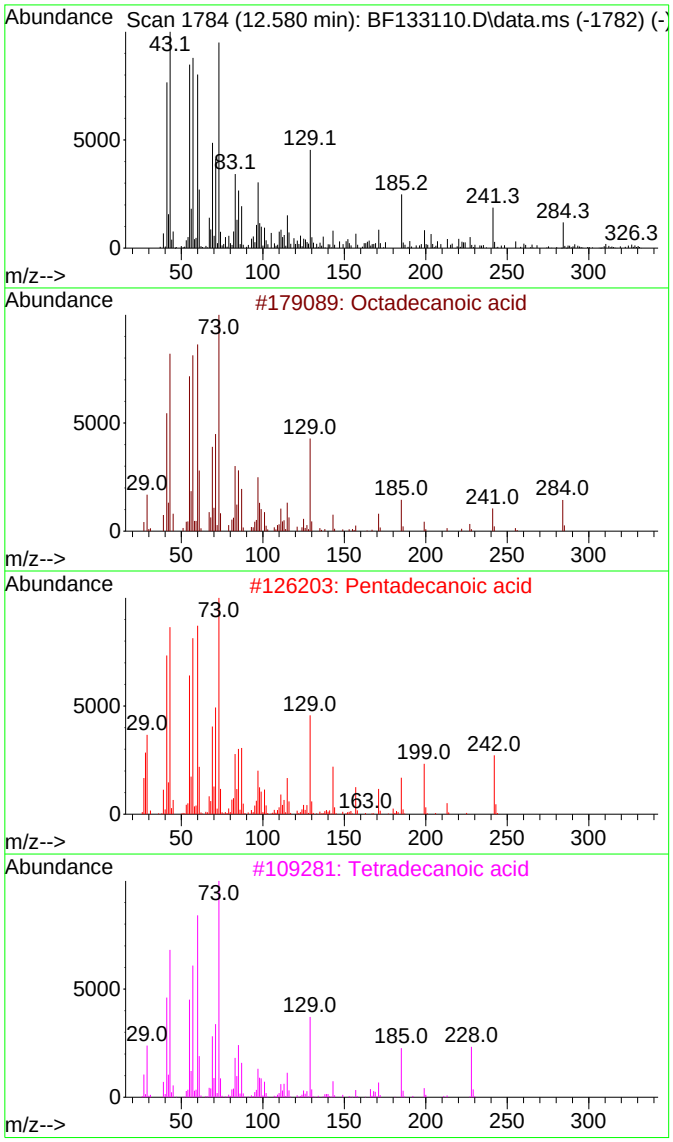
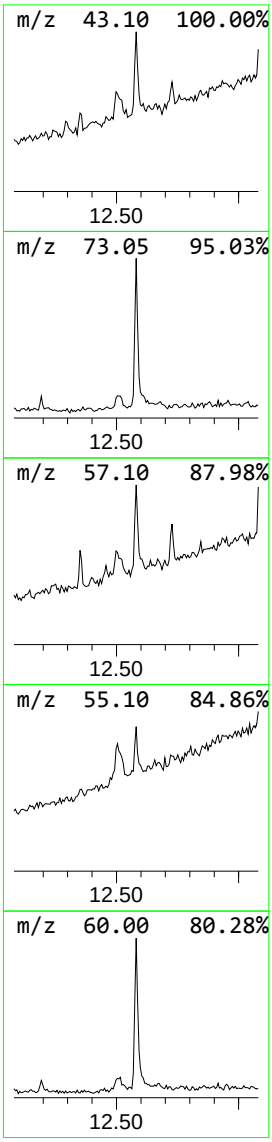
Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.580	4.17 ng	347681	Chrysene-d12	13.892

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	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133110.D
Acq On : 27 Apr 2023 20:27
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

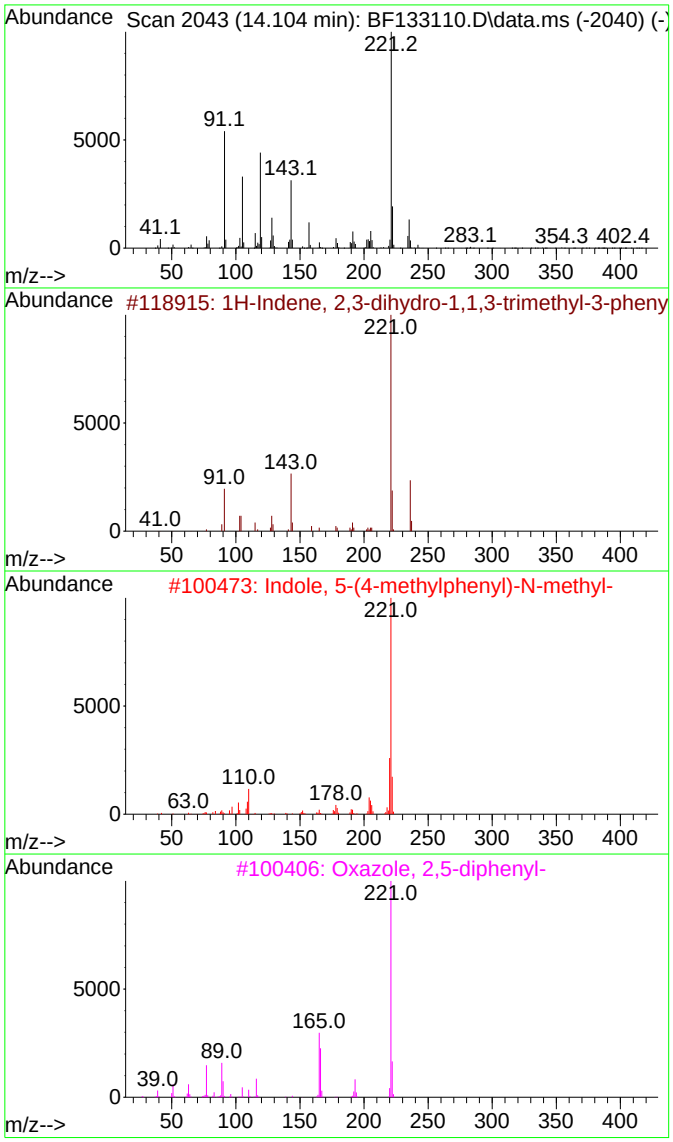
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

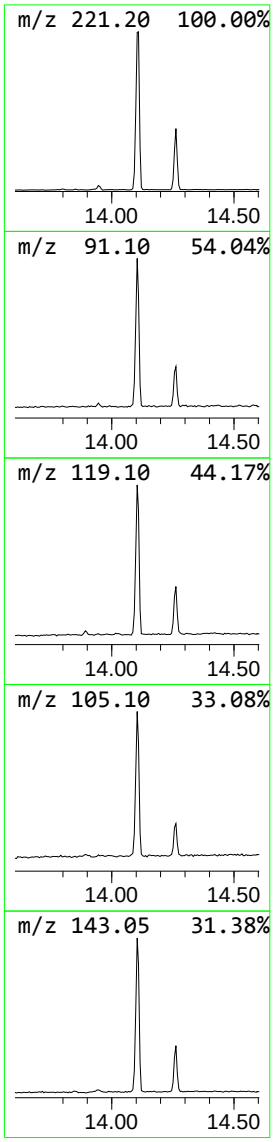
****

Peak Number 5 unknown14.104 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.104	33.95 ng	2829500	Chrysene-d12	13.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	47
2	Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	43
3	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	38
4	2,3-Dihydro-2-methyl-4-phenyl-1H...	236	C16H16N2	111536-73-3	38
5	1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
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Acq On : 27 Apr 2023 20:27
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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

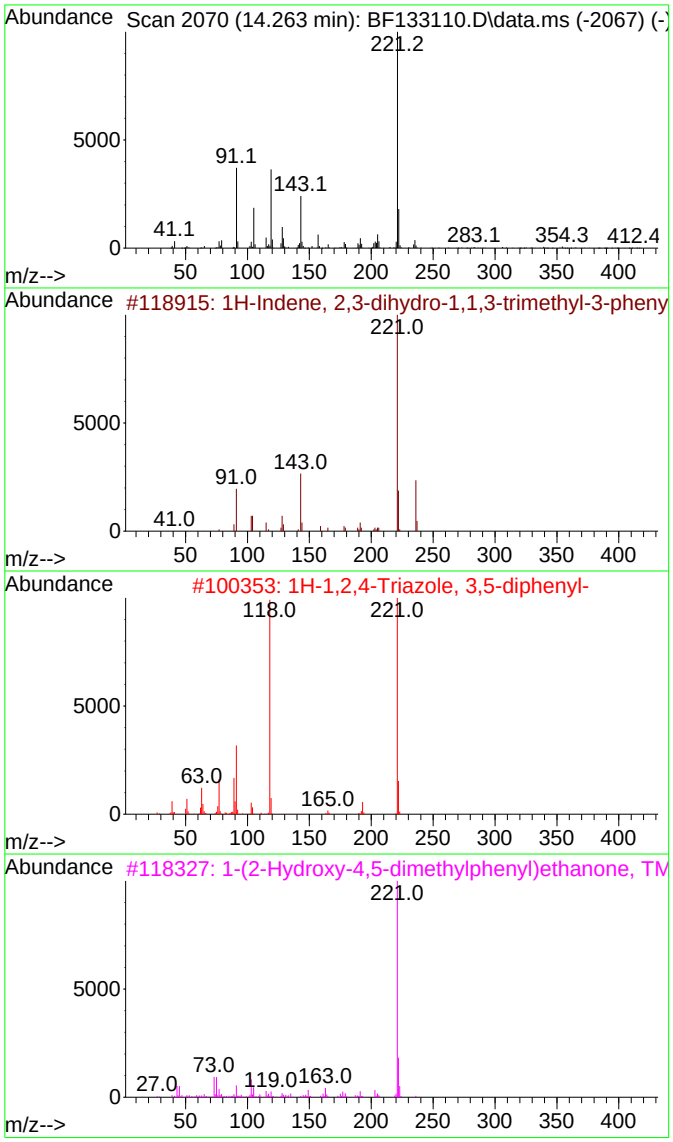
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

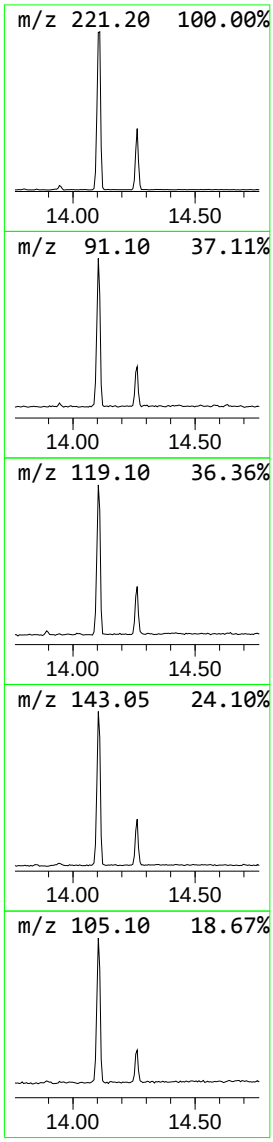
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.263	8.45 ng	704029	Chrysene-d12	13.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	64
2	1H-1,2,4-Triazole, 3,5-diphenyl-	221	C14H11N3	002039-06-7	47
3	1-(2-Hydroxy-4,5-dimethylphenyl)...	236	C13H20O2Si	1000484-73-7	47
4	N-Methyl-m-hemipimide	221	C11H11NO4	092288-92-1	47
5	1-(2-Hydroxy-5-methylphenyl)prop...	236	C13H20O2Si	1000506-71-9	47





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

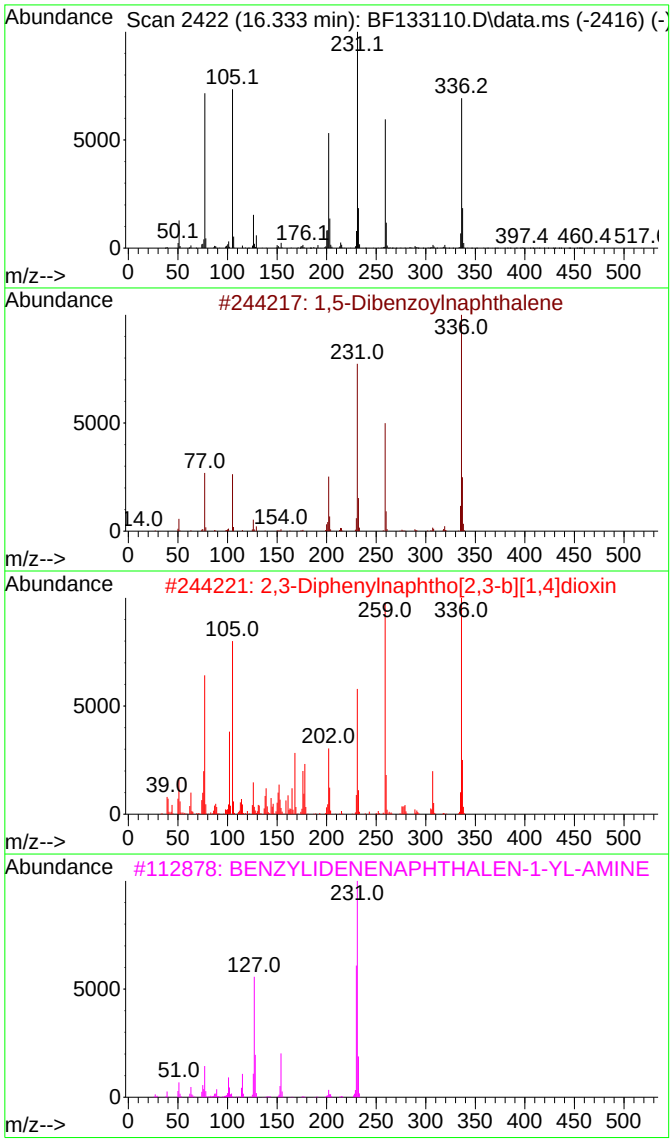
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

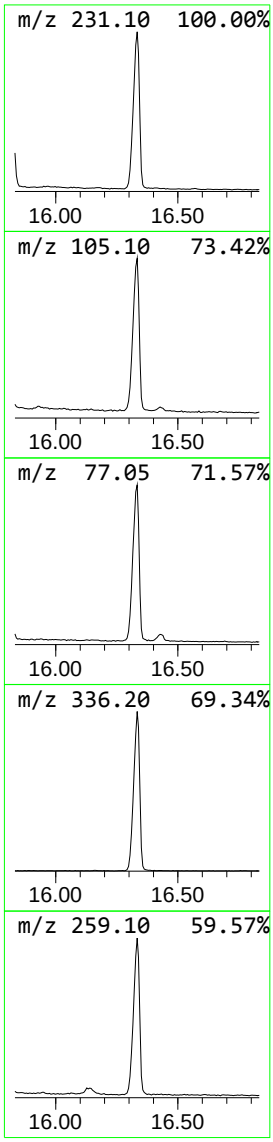
****

Peak Number 7 1,5-Dibenzoylnaphthalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.333	93.49 ng	3654530	Perylene-d12	15.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5-Dibenzoylnaphthalene	336	C24H16O2	000083-80-7	99
2	2,3-Diphenylnaphtho[2,3-b][1,4]d...	336	C24H16O2	091201-57-9	52
3	BENZYLIDENENAPHTHALEN-1-YL-AMINE	231	C17H13N	000890-51-7	38
4	1-Benzoyl-2-t-butyl-5-ethyl-3-me...	288	C17H24N2O2	109918-66-3	27
5	Cyclohexanamine, 2-[(phenylethyn...	231	C14H17NS	1000327-34-1	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133110.D
Acq On : 27 Apr 2023 20:27
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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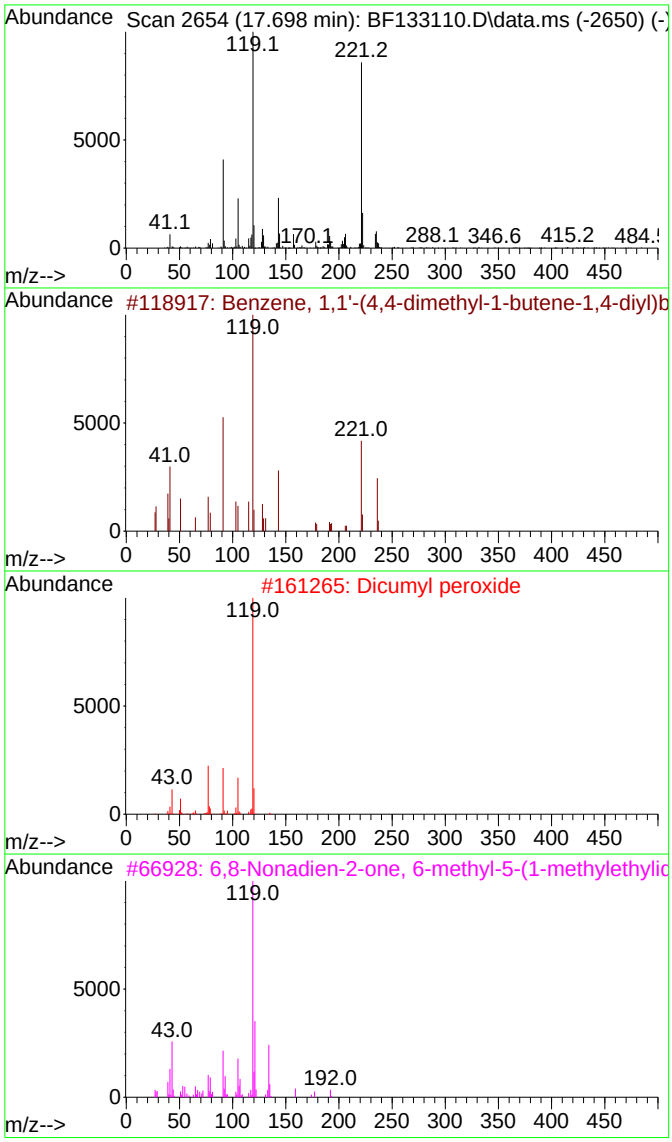
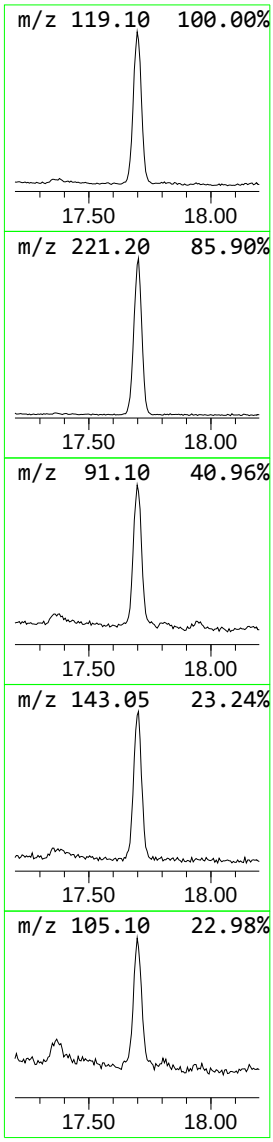
Peak Number 8 unknown17.698 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.698	22.95 ng	897347	Perylene-d12	15.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(4,4-dimethyl-1-bu...	236	C18H20	093393-51-2	47
2	Dicumyl peroxide	270	C18H22O2	000080-43-3	35
3	6,8-Nonadien-2-one, 6-methyl-5-(...	192	C13H20O	060714-16-1	35
4	3,5,5,9-Tetramethyl-4a,5,6,7,8,9...	204	C15H24	1000412-94-8	35
5	Carbonic acid, monoamide, N-(2-e...	221	C13H19NO2	1000339-98-3	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133110.D
Acq On : 27 Apr 2023 20:27
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Diallyl phthalate	10.904	6.5	ng	821987	4	11.251	2532500	20.0
n-Hexadecanoic ...	11.792	6.7	ng	850172	4	11.251	2532500	20.0
9,10-Anthracene...	12.069	2.7	ng	337290	4	11.251	2532500	20.0
Octadecanoic acid	12.580	4.2	ng	347681	5	13.892	1666830	20.0
unknown14.104	14.104	34.0	ng	2829500	5	13.892	1666830	20.0
1H-Indene, 2,3-...	14.263	8.4	ng	704029	5	13.892	1666830	20.0
1,5-Dibenzoylna...	16.333	93.5	ng	3654530	6	15.333	781842	20.0
unknown17.698	17.698	22.9	ng	897347	6	15.333	781842	20.0