

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
 Data File : BF132985.D
 Acq On : 21 Apr 2023 23:42
 Operator : CG\JU
 Sample : 02389-23 2X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SPB-6WC-23-04-17

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: BF132985.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.740	273	281	288	rBV	48526	76950	3.60%	0.244%
2	4.357	382	386	395	rVB3	31270	46444	2.18%	0.147%
3	4.934	481	484	491	rVB	65569	77351	3.62%	0.246%
4	5.216	528	532	535	rVB	55709	48723	2.28%	0.155%
5	5.328	547	551	553	rBV	216775	240374	11.26%	0.763%
6	5.357	553	556	560	rVB	2354237	2020365	94.64%	6.416%
7	5.587	589	595	600	rBV	187493	180941	8.48%	0.575%
8	6.351	720	725	727	rBV3	42208	52083	2.44%	0.165%
9	6.387	727	731	734	rVV	2469771	2023617	94.80%	6.426%
10	6.440	736	740	747	rBV5	29343	56233	2.63%	0.179%
11	6.522	750	754	761	rVB3	55798	58676	2.75%	0.186%
12	6.581	761	764	765	rBV	68561	61687	2.89%	0.196%
13	6.751	789	793	796	rBV	1680273	1304089	61.09%	4.141%
14	6.810	801	803	812	rBV3	32157	65513	3.07%	0.208%
15	7.151	858	861	864	rBV2	51177	61566	2.88%	0.196%
16	7.310	881	888	891	rBV	1561338	1252617	58.68%	3.978%
17	7.357	894	896	900	rVB	71118	56611	2.65%	0.180%
18	7.398	900	903	911	rBV5	35797	51647	2.42%	0.164%
19	8.034	1008	1011	1014	rBV	2040829	1691904	79.26%	5.373%
20	8.057	1014	1015	1017	rVB	197801	90959	4.26%	0.289%
21	8.634	1110	1113	1116	rVB	70323	50873	2.38%	0.162%
22	8.745	1130	1132	1136	rVB	128616	100706	4.72%	0.320%
23	8.792	1136	1140	1146	rBV	77382	104725	4.91%	0.333%
24	8.845	1146	1149	1152	rVV	80326	62703	2.94%	0.199%
25	9.063	1184	1186	1191	rVB2	51883	48122	2.25%	0.153%
26	9.110	1191	1194	1197	rBV	2863155	2134727	100.00%	6.779%
27	9.198	1203	1209	1213	rBV4	146501	260715	12.21%	0.828%
28	9.304	1225	1227	1232	rVB3	42134	47974	2.25%	0.152%
29	9.375	1235	1239	1242	rBV2	53833	75568	3.54%	0.240%
30	9.451	1249	1252	1254	rBV2	71524	68374	3.20%	0.217%
31	9.498	1258	1260	1262	rBV2	81859	72985	3.42%	0.232%
32	9.651	1283	1286	1290	rBV2	63809	92074	4.31%	0.292%
33	9.704	1293	1295	1297	rVB2	70479	51763	2.42%	0.164%
34	9.728	1297	1299	1304	rBV3	87262	102146	4.78%	0.324%
35	9.786	1304	1309	1312	rBV	1917827	1615678	75.69%	5.131%
36	9.822	1312	1315	1322	rVB	268155	290326	13.60%	0.922%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
 Data File : BF132985.D
 Acq On : 21 Apr 2023 23:42
 Operator : CG\JU
 Sample : 02389-23 2X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SPB-6WC-23-04-17

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	9.992	1341	1344	1347	rVB	150589	118683	5.56%	0.377%
38	10.198	1376	1379	1382	rBV	312476	252064	11.81%	0.800%
39	10.333	1400	1402	1406	rVB	169173	127489	5.97%	0.405%
40	10.428	1414	1418	1427	rBV2	1084367	1814483	85.00%	5.762%
41	10.575	1440	1443	1448	rBV	1037809	1017652	47.67%	3.232%
42	10.616	1448	1450	1453	rVV	188546	146419	6.86%	0.465%
43	10.716	1462	1467	1473	rBV4	157144	286047	13.40%	0.908%
44	10.828	1484	1486	1488	rBV2	91863	87425	4.10%	0.278%
45	10.880	1493	1495	1498	rBV2	232856	206025	9.65%	0.654%
46	11.275	1558	1562	1563	rBV	1337686	1246708	58.40%	3.959%
47	11.298	1563	1566	1569	rVV	1788660	1598235	74.87%	5.075%
48	11.345	1571	1574	1577	rVB	486253	395213	18.51%	1.255%
49	11.804	1649	1652	1653	rBV	347715	361820	16.95%	1.149%
50	11.880	1663	1665	1669	rBV2	311748	358935	16.81%	1.140%
51	12.486	1765	1768	1771	rVB	2280956	2125989	99.59%	6.751%
52	12.716	1804	1807	1810	rVB	1977069	1778465	83.31%	5.648%
53	12.863	1829	1832	1838	rVB	1534565	1483843	69.51%	4.712%
54	13.910	2007	2010	2013	rBV3	1468411	1824377	85.46%	5.793%
55	14.127	2044	2047	2055	rVB	1553027	1563505	73.24%	4.965%

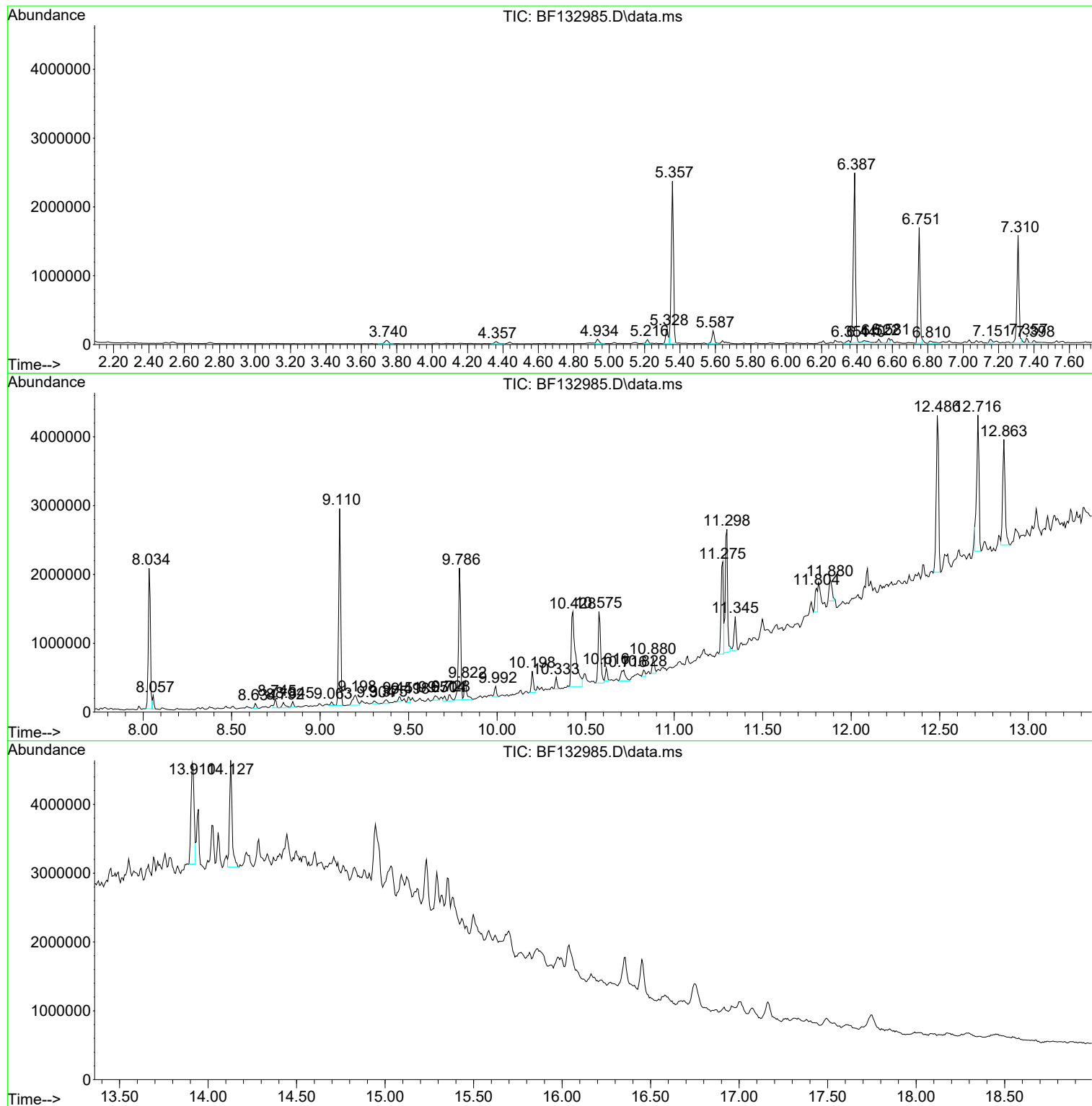
Sum of corrected areas: 31491186

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132985.D
Acq On : 21 Apr 2023 23:42
Operator : CG\JU
Sample : 02389-23 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-6WC-23-04-17

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\BF042123\
Data File : BF132985.D
Acq On : 21 Apr 2023 23:42
Operator : CG\JU
Sample : 02389-23 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-6WC-23-04-17

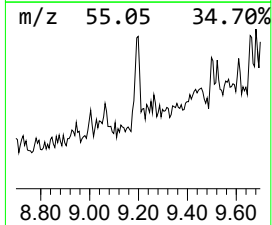
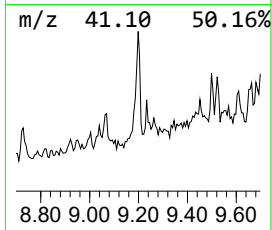
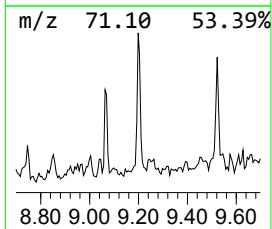
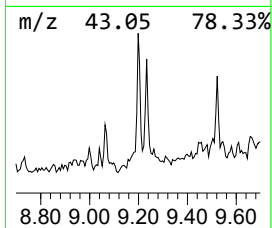
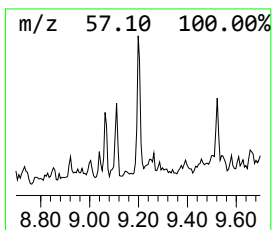
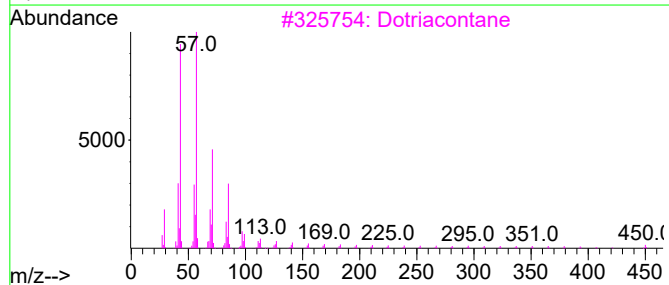
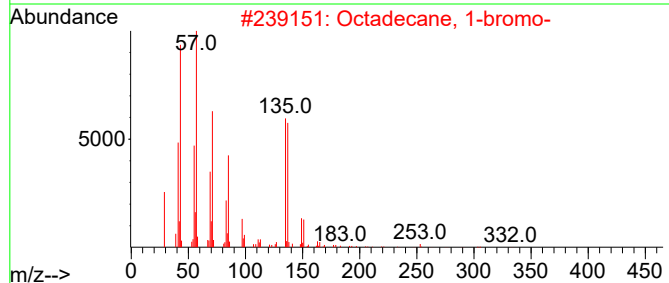
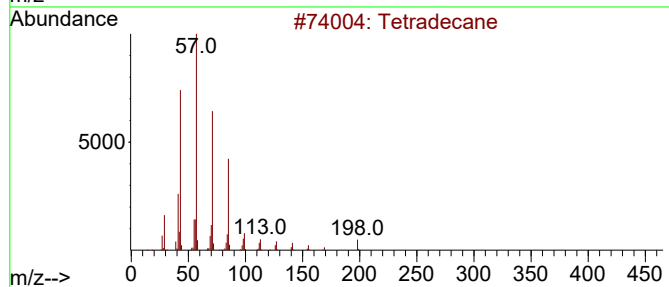
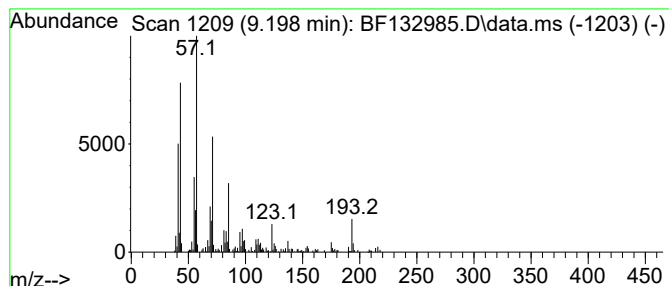
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.198	3.23 ng	260715	Acenaphthene-d10	9.786

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	64
2		Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	52
3		Dotriacontane	451	C32H66	000544-85-4	52
4		Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	47
5		Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132985.D
Acq On : 21 Apr 2023 23:42
Operator : CG\JU
Sample : 02389-23 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-6WC-23-04-17

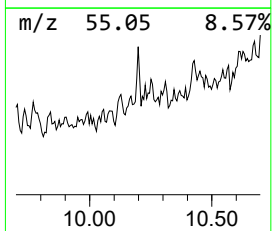
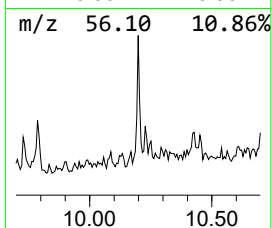
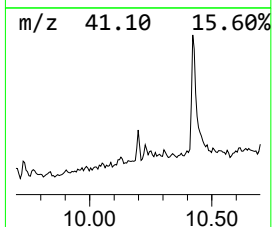
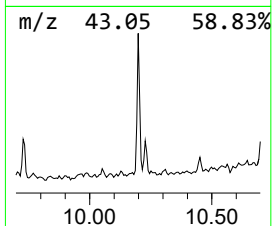
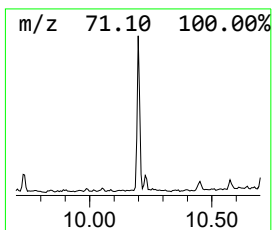
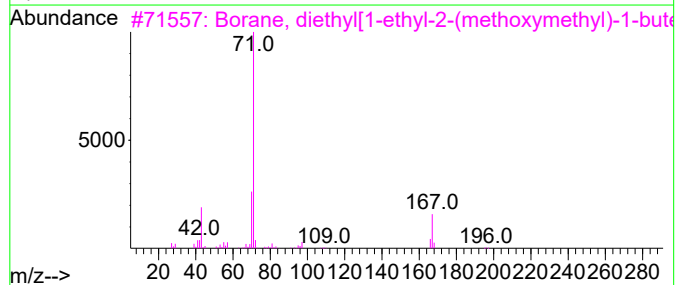
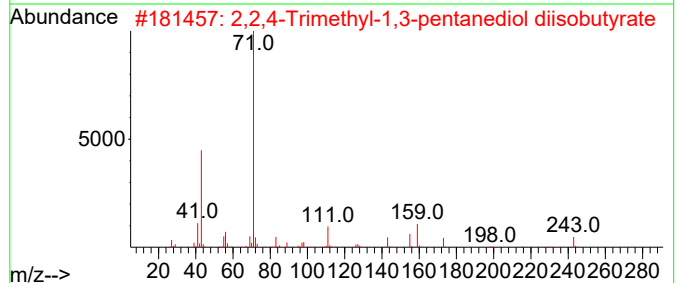
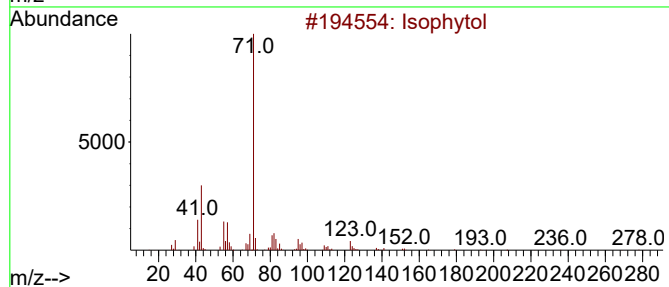
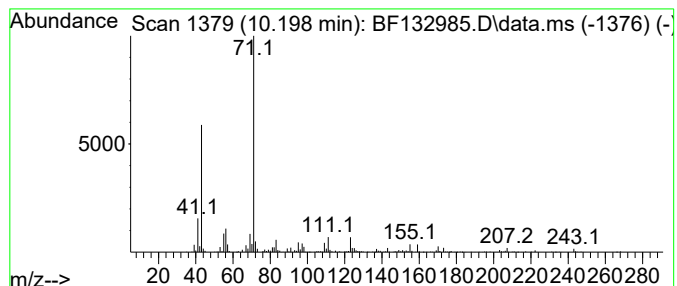
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Isophytol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.198	3.12 ng	252064	Acenaphthene-d10	9.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isophytol	296	C20H40O	000505-32-8	72
2			2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
3			Borane, diethyl[1-ethyl-2-(metho...	196	C12H25BO	053670-48-7	59
4			Tetrahydrofurfuryl chloride	120	C5H9ClO	003003-84-7	53
5			Diethylmalonic acid, monochlorid...	262	C12H19ClO4	1000370-65-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132985.D
Acq On : 21 Apr 2023 23:42
Operator : CG\JU
Sample : 02389-23 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-6WC-23-04-17

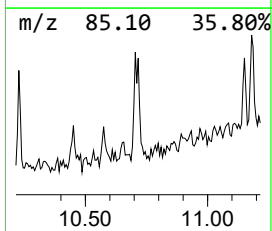
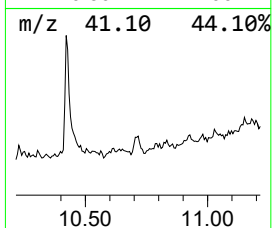
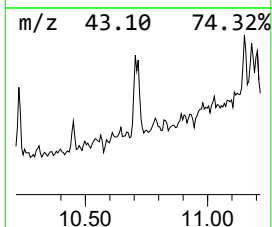
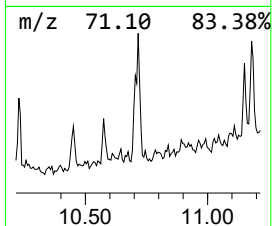
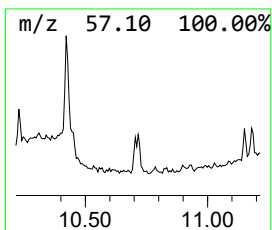
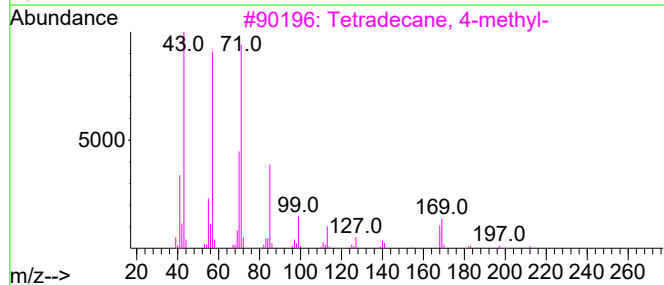
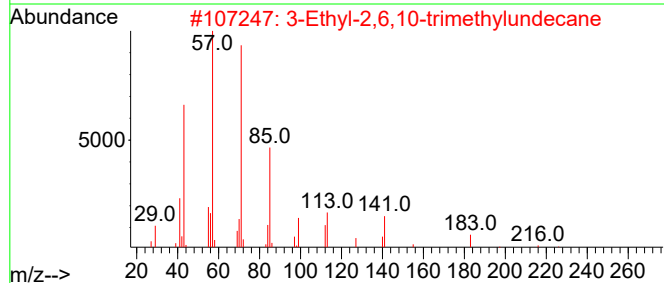
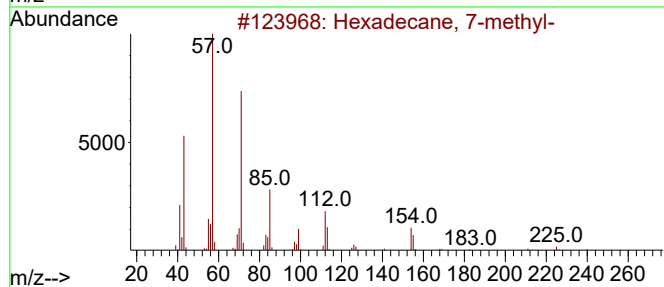
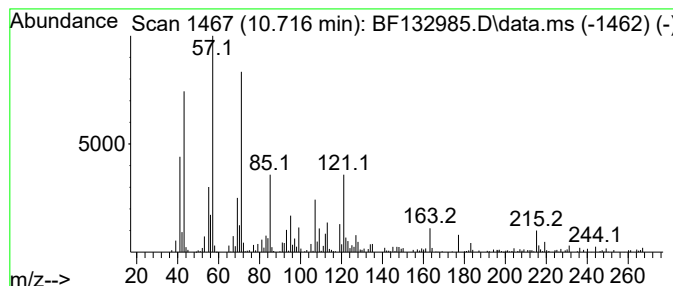
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane, 7-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.716	4.59 ng	286047	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 7-methyl-	240	C17H36	026730-20-1	78
2			3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	78
3			Tetradecane, 4-methyl-	212	C15H32	025117-24-2	78
4			Tridecane, 5-propyl-	226	C16H34	055045-11-9	60
5			Undecane, 6-ethyl-	184	C13H28	017312-60-6	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132985.D
Acq On : 21 Apr 2023 23:42
Operator : CG\JU
Sample : 02389-23 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-6WC-23-04-17

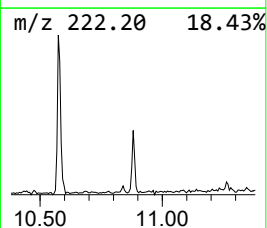
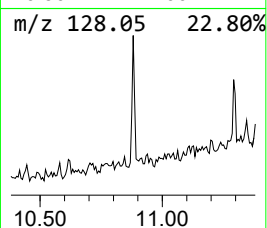
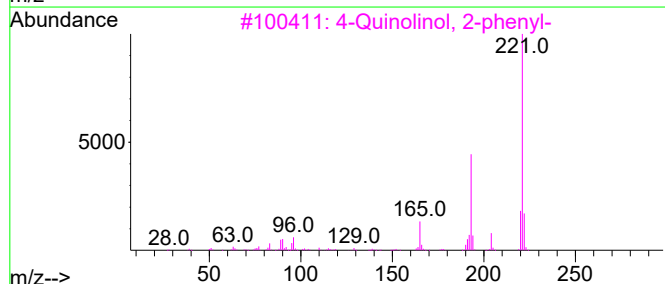
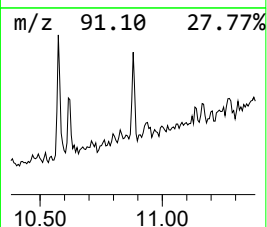
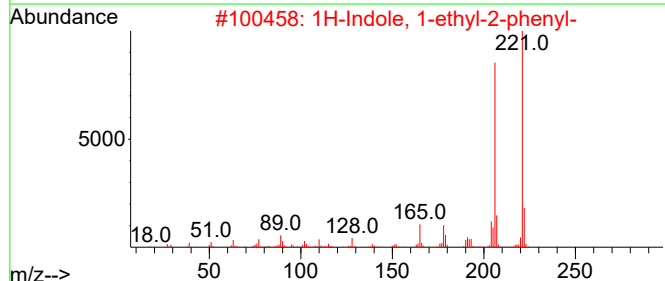
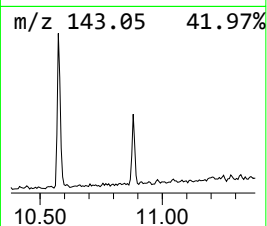
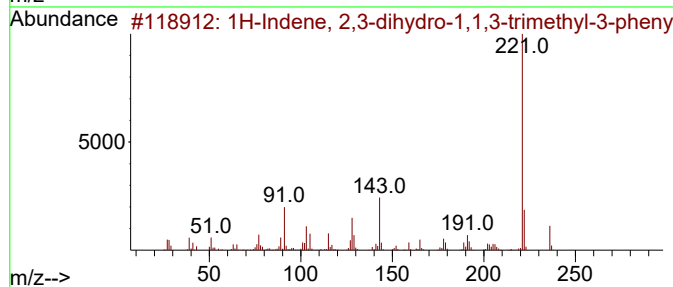
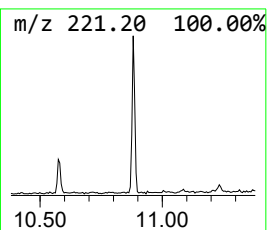
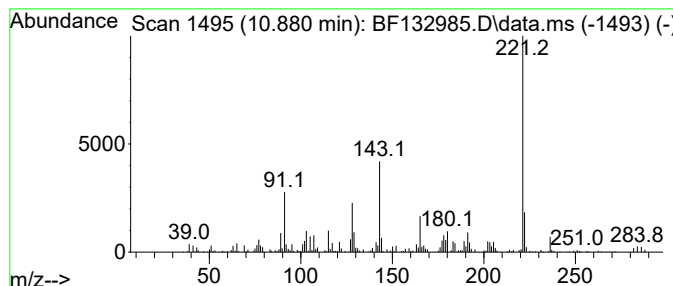
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.881	3.31 ng	206025	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	93
2			1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	49
3			4-Quinolinol, 2-phenyl-	221	C15H11NO	001144-20-3	46
4			4-Hydroxy-beta-phenylcinnamionitrile	221	C15H11NO	016281-90-6	43
5			1H-Quinolin-2-one, 3-phenyl-	221	C15H11NO	038035-81-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132985.D
Acq On : 21 Apr 2023 23:42
Operator : CG\JU
Sample : 02389-23 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

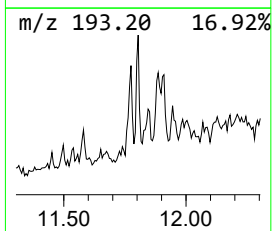
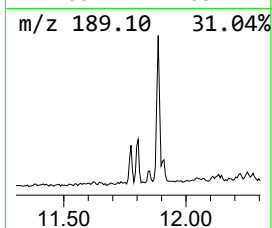
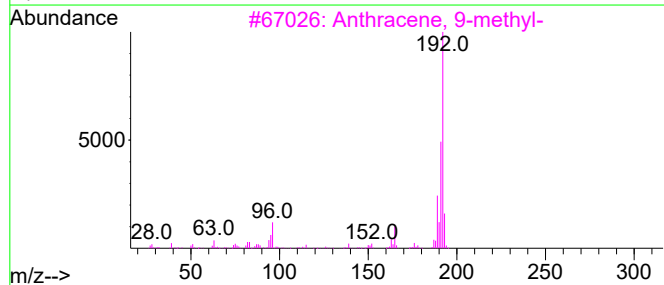
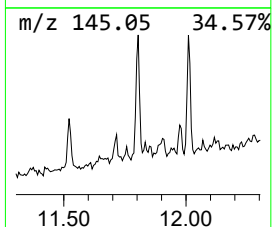
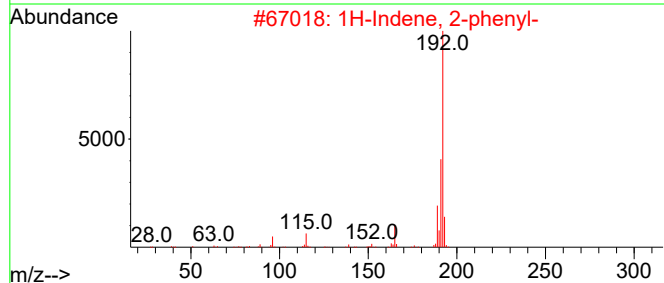
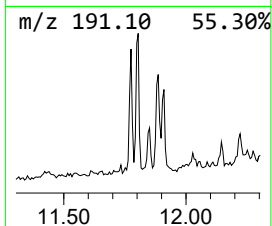
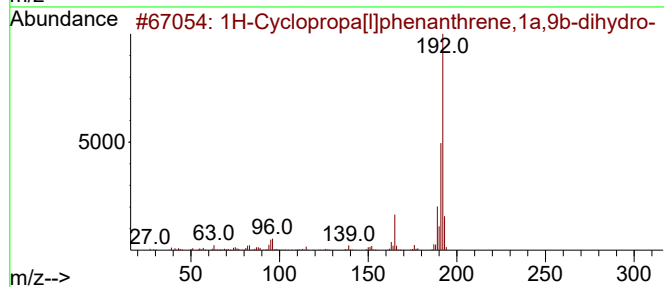
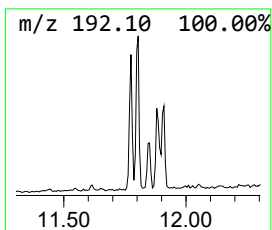
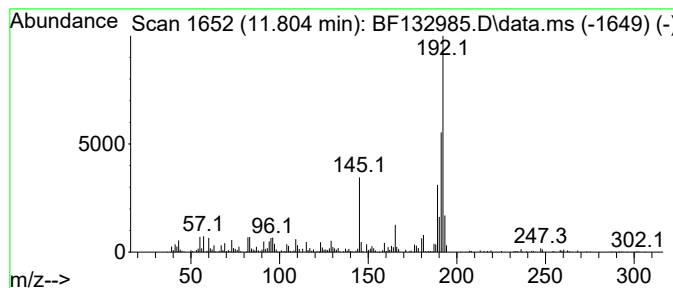
Instrument :
BNA_F
ClientSampleId :
SPB-6WC-23-04-17

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-Cyclopropa[l]phenanthren... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.804	5.80 ng	361820	Phenanthrene-d10		11.275	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Cyclopropa[1]phenanthrene,1a,...		192	C15H12	000949-41-7	94
2	1H-Indene, 2-phenyl-		192	C15H12	004505-48-0	93
3	Anthracene, 9-methyl-		192	C15H12	000779-02-2	93
4	Phenanthrene, 4-methyl-		192	C15H12	000832-64-4	93
5	Phenanthrene, 3-methyl-		192	C15H12	000832-71-3	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132985.D
Acq On : 21 Apr 2023 23:42
Operator : CG\JU
Sample : 02389-23 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-6WC-23-04-17

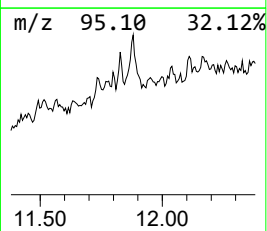
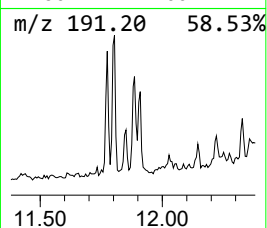
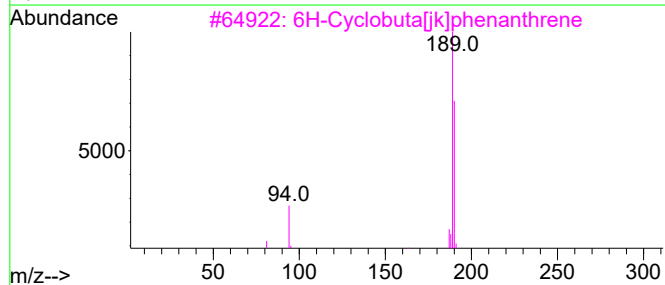
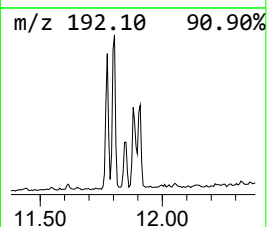
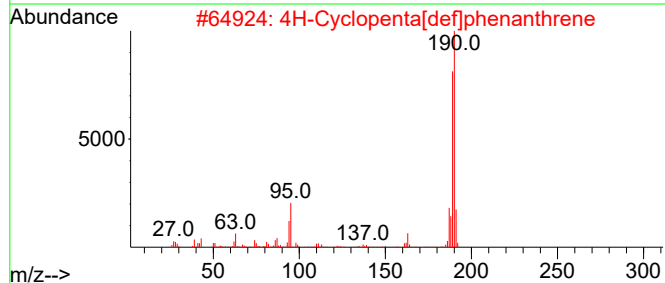
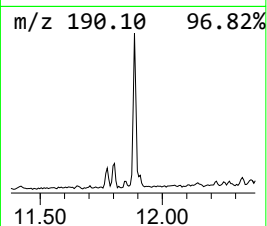
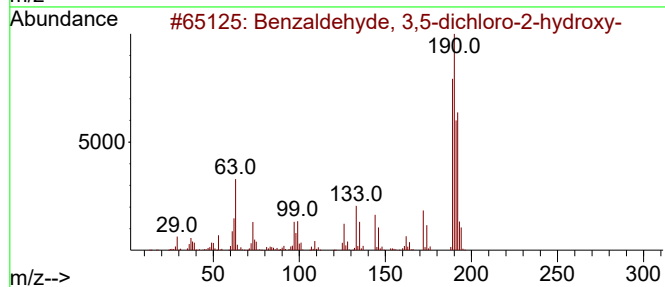
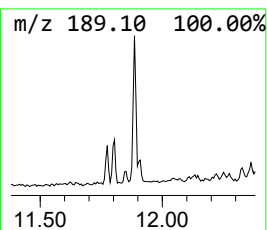
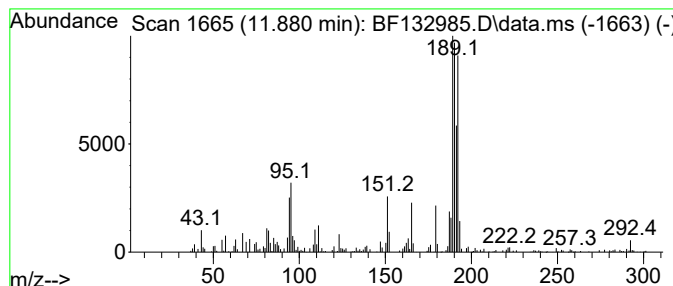
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzaldehyde, 3,5-dichloro-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	5.76 ng	358935	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	58
2			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	55
3			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	43
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132985.D
Acq On : 21 Apr 2023 23:42
Operator : CG\JU
Sample : 02389-23 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-6WC-23-04-17

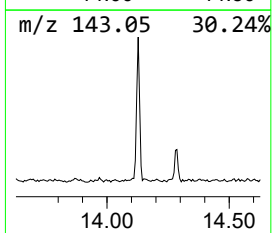
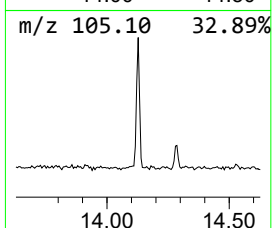
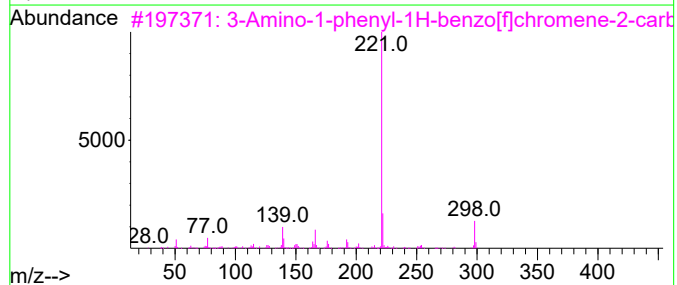
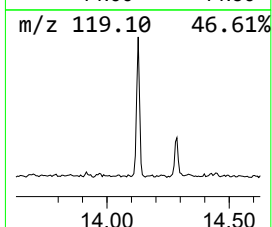
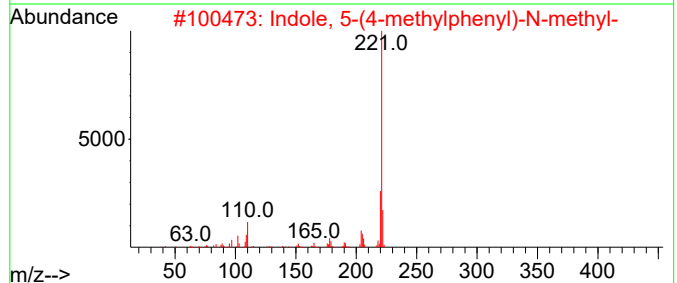
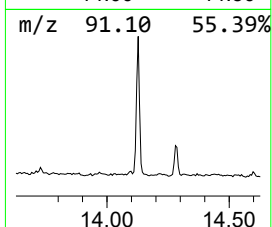
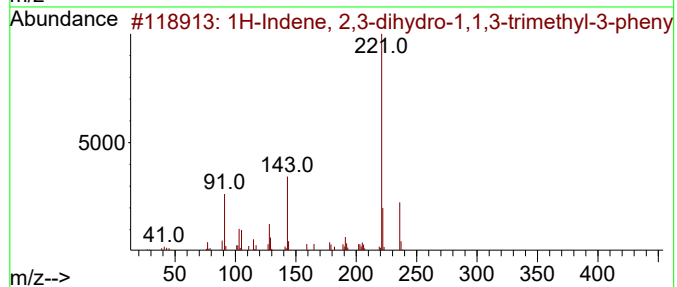
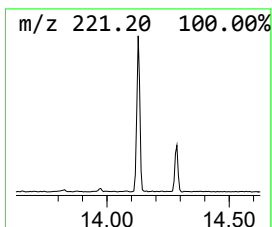
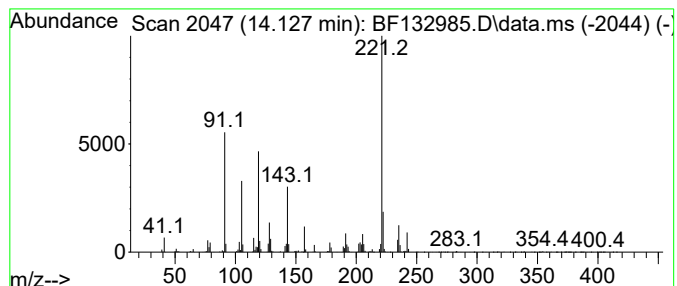
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.127 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.127	17.14 ng	1563510	Chrysene-d12	13.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	50		
2	Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	43		
3	3-Amino-1-phenyl-1H-benzo[f]chro...	298	C20H14N2O	111861-46-2	38		
4	(Dimethylphenylsilyl)phenylacety...	236	C16H16Si	1000434-31-1	38		
5	2-Mercapto-4,6-dimethylnicotinon...	236	C11H16N2SSi	1000332-43-1	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132985.D
Acq On : 21 Apr 2023 23:42
Operator : CG\JU
Sample : 02389-23 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-6WC-23-04-17

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Tetradecane	9.198	3.2	ng	260715	3	9.786	1615680	20.0
Isophytol	10.198	3.1	ng	252064	3	9.786	1615680	20.0
Hexadecane, 7-m...	10.716	4.6	ng	286047	4	11.275	1246710	20.0
1H-Indene, 2,3-...	10.881	3.3	ng	206025	4	11.275	1246710	20.0
1H-Cyclopropa[1...	11.804	5.8	ng	361820	4	11.275	1246710	20.0
Benzaldehyde, 3...	11.880	5.8	ng	358935	4	11.275	1246710	20.0
unknown14.127	14.127	17.1	ng	1563510	5	13.916	1824380	20.0