

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
 Data File : BF134353.D
 Acq On : 18 Jul 2023 23:34
 Operator : CG\JU
 Sample : 03601-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-1-071223

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	506	508	520	rVB	27760	36878	2.44%	0.317%
2	5.469	571	575	584	rBV	1310256	1292871	85.71%	11.112%
3	5.863	635	642	645	rVB4	13005	20931	1.39%	0.180%
4	6.087	674	680	686	rBV7	20992	37438	2.48%	0.322%
5	6.269	705	711	715	rVB4	15252	20953	1.39%	0.180%
6	6.363	724	727	733	rBV4	27192	34046	2.26%	0.293%
7	6.481	743	747	758	rBV	1335070	1270341	84.22%	10.918%
8	6.669	775	779	784	rBV3	47421	62526	4.15%	0.537%
9	6.834	804	807	811	rBV	415115	376985	24.99%	3.240%
10	7.104	847	853	856	rVB4	17224	21143	1.40%	0.182%
11	7.398	899	903	906	rBV	893921	807417	53.53%	6.940%
12	7.475	911	916	919	rVB7	16305	19582	1.30%	0.168%
13	8.116	1021	1025	1028	rBV	572620	437753	29.02%	3.762%
14	8.528	1092	1095	1097	rBV	21936	19339	1.28%	0.166%
15	9.128	1195	1197	1204	rBV3	29358	32155	2.13%	0.276%
16	9.192	1204	1208	1211	rBV	1952779	1508350	100.00%	12.964%
17	9.269	1217	1221	1223	rVB4	24164	22740	1.51%	0.195%
18	9.304	1223	1227	1231	rBV3	33364	36135	2.40%	0.311%
19	9.528	1262	1265	1268	rBV3	20078	21502	1.43%	0.185%
20	9.586	1274	1275	1278	rVB	29236	19975	1.32%	0.172%
21	9.733	1297	1300	1303	rBV2	25761	24062	1.60%	0.207%
22	9.875	1320	1324	1327	rVB	480119	430538	28.54%	3.700%
23	10.075	1357	1358	1363	rVB5	19470	19431	1.29%	0.167%
24	10.116	1363	1365	1370	rBV3	15804	19137	1.27%	0.164%
25	10.275	1389	1392	1394	rBV3	19249	19760	1.31%	0.170%
26	10.422	1414	1417	1423	rBV2	21532	22598	1.50%	0.194%
27	10.522	1431	1434	1440	rVB	27008	34315	2.28%	0.295%
28	10.669	1455	1459	1465	rBV	896930	827628	54.87%	7.113%
29	10.786	1474	1479	1487	rVB	50942	70567	4.68%	0.607%
30	11.257	1556	1559	1564	rVB4	36975	49042	3.25%	0.422%
31	11.369	1574	1578	1580	rBV	487226	428406	28.40%	3.682%
32	11.392	1580	1582	1585	rVV	164319	129019	8.55%	1.109%
33	11.439	1588	1590	1593	rVB	31183	28298	1.88%	0.243%
34	11.610	1615	1619	1622	rBV5	16664	23431	1.55%	0.201%
35	11.869	1661	1663	1665	rBV	25767	24990	1.66%	0.215%
36	11.898	1665	1668	1675	rVB2	276939	259605	17.21%	2.231%

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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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.980	1680	1682	1685	rVV	49074	55213	3.66%	0.475%
38	12.010	1685	1687	1690	rVB2	25540	21797	1.45%	0.187%
39	12.351	1742	1745	1747	rBV3	17021	20468	1.36%	0.176%
40	12.422	1755	1757	1760	rBV	22799	22558	1.50%	0.194%
41	12.469	1760	1765	1770	rVB6	36416	60401	4.00%	0.519%
42	12.592	1782	1786	1788	rBV	249084	233709	15.49%	2.009%
43	12.686	1800	1802	1806	rBV	90887	88427	5.86%	0.760%
44	12.822	1819	1825	1830	rBV	228480	272456	18.06%	2.342%
45	12.963	1845	1849	1853	rBV	1503787	1365518	90.53%	11.736%
46	14.033	2026	2031	2034	rBV2	404623	472876	31.35%	4.064%
47	14.127	2044	2047	2051	rVB	249144	230858	15.31%	1.984%
48	15.545	2285	2288	2293	rVB	221633	280901	18.62%	2.414%

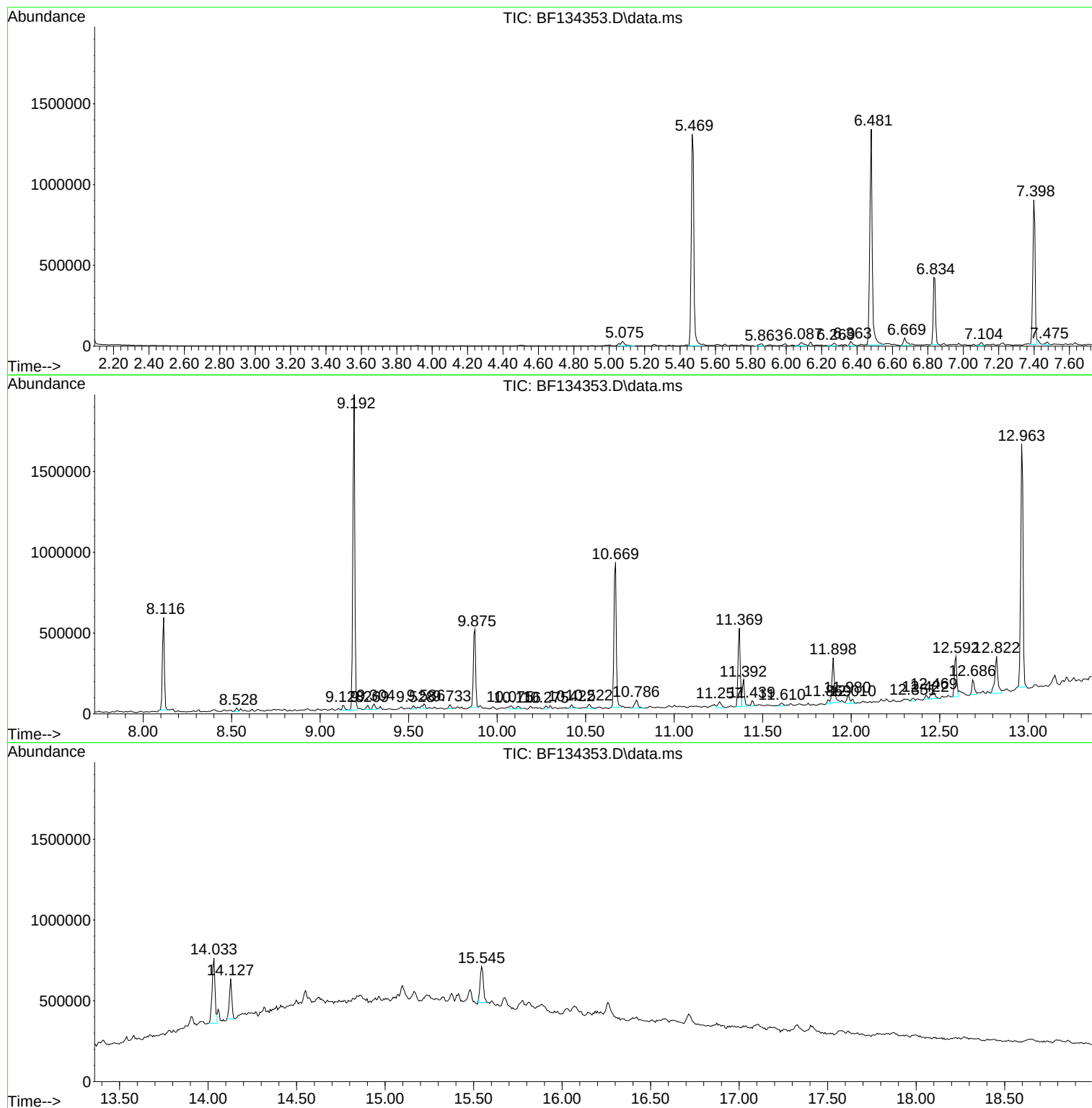
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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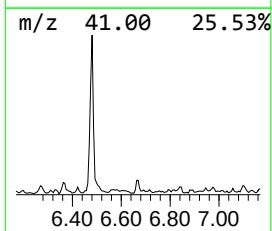
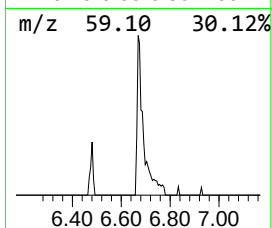
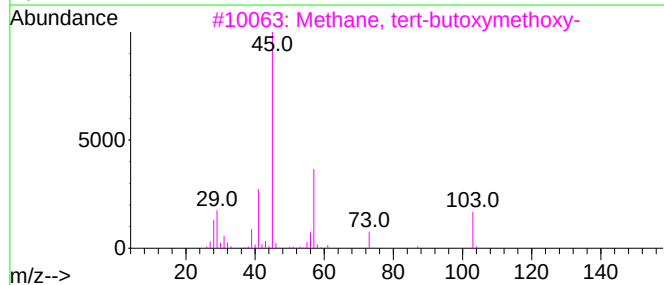
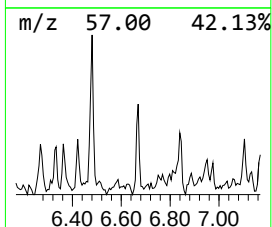
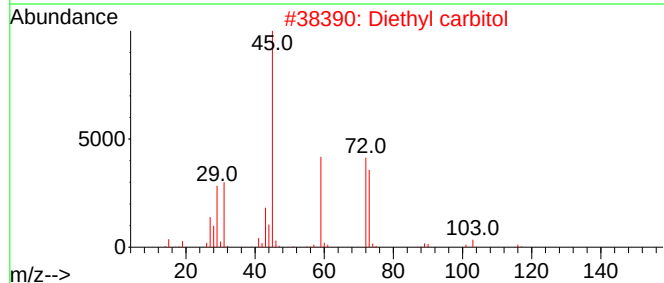
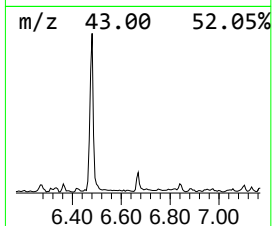
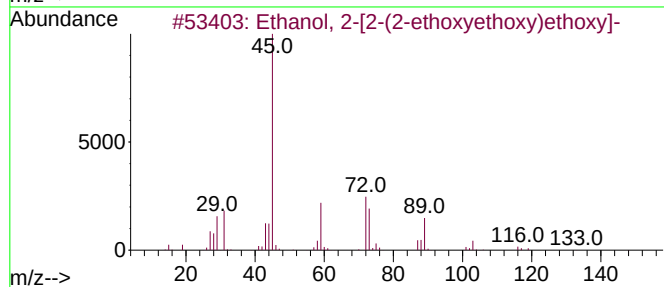
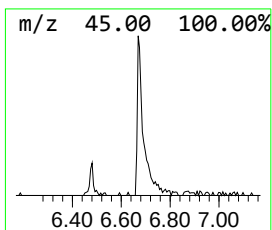
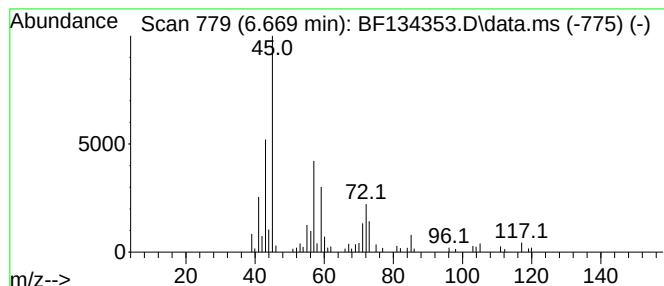
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-[2-(2-ethoxyetho... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.669	3.32 ng	62526	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	59
2			Diethyl carbitol	162	C8H18O3	000112-36-7	59
3			Methane, tert-butoxymethoxy-	118	C6H14O2	024209-75-4	47
4			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	45
5			1-Butene, 4-methoxy	86	C5H10O	004696-30-4	43



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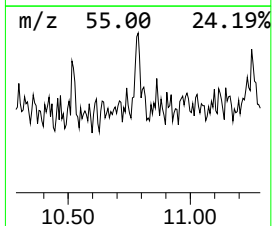
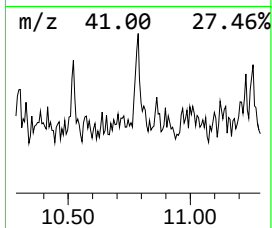
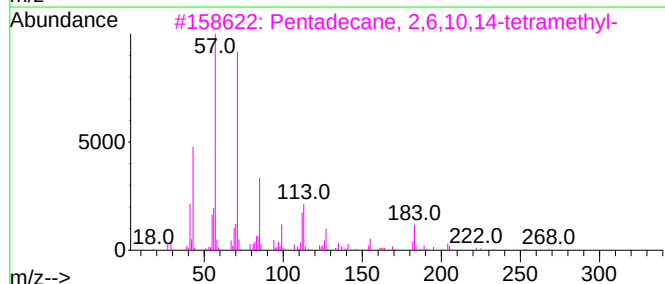
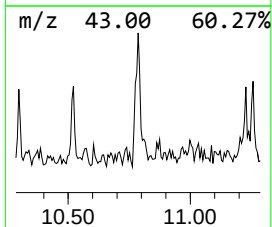
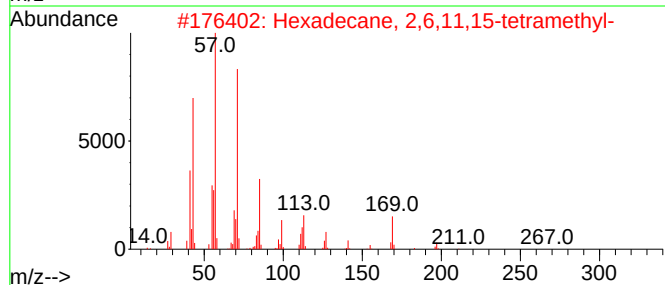
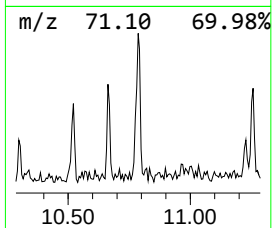
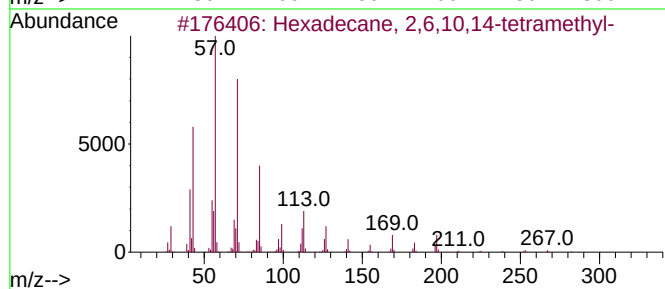
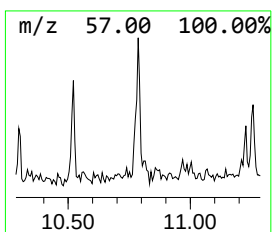
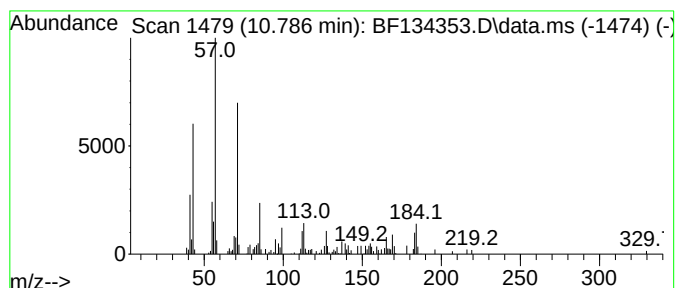
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecane, 2,6,10,14-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.786	3.29 ng	70567	Phenanthrene-d10	11.369	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64
2	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	64
3	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	64
4	Nonane, 5-propyl-	170	C12H26	000998-35-6	55
5	Decane, 2-methyl-	156	C11H24	006975-98-0	52



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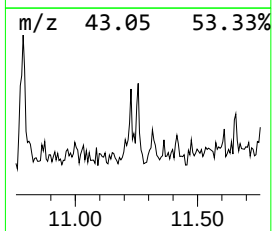
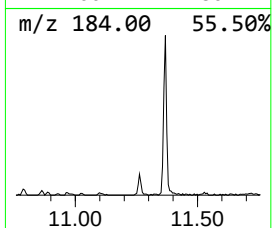
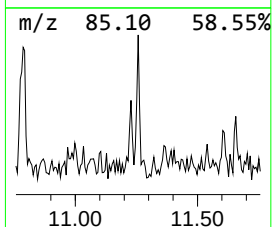
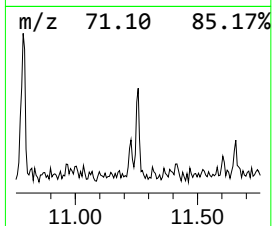
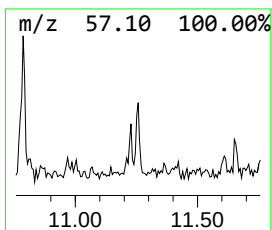
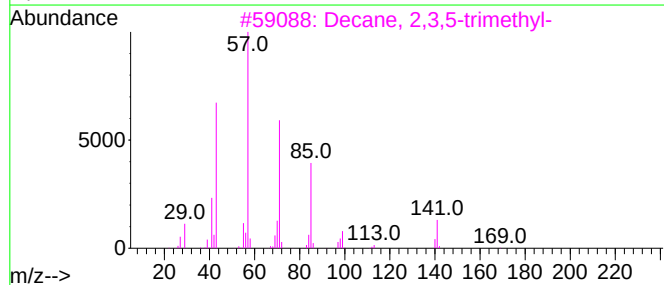
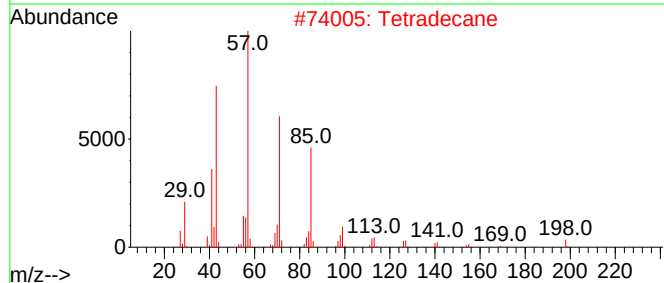
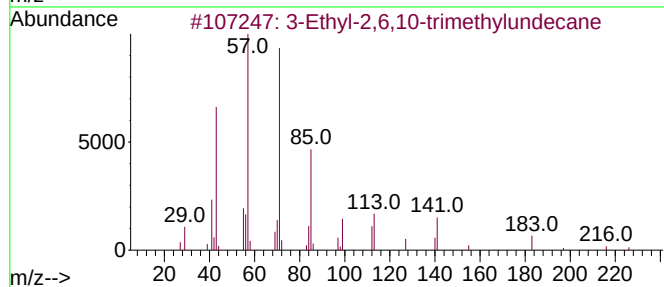
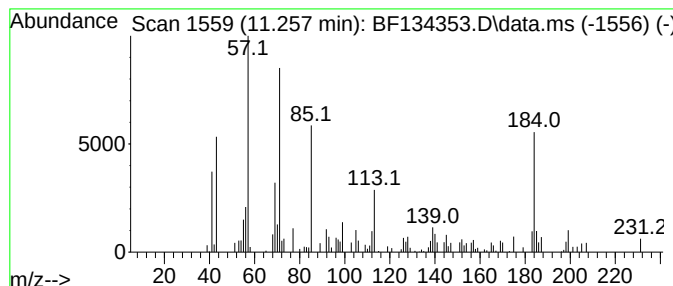
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown11.257 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.257	2.29 ng	49042	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	49
2			Tetradecane	198	C14H30	000629-59-4	49
3			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	43
4			4-Octanone	128	C8H16O	000589-63-9	43
5			Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	38



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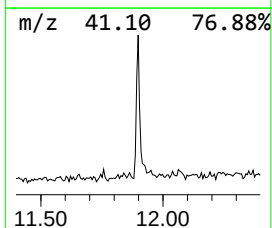
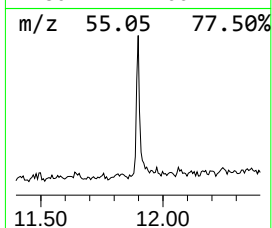
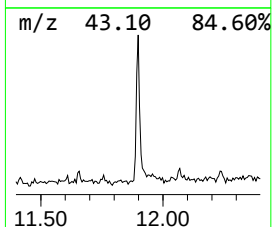
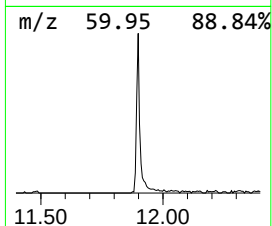
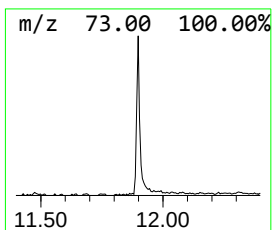
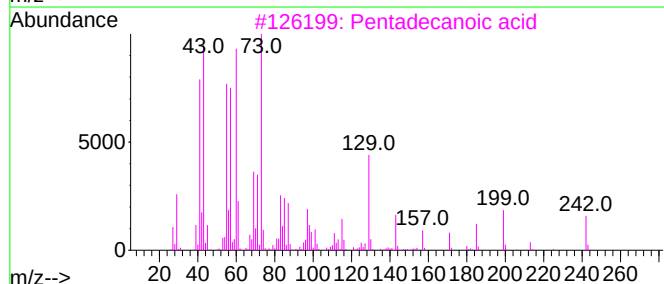
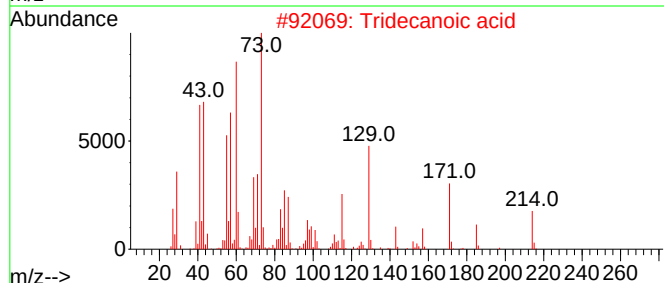
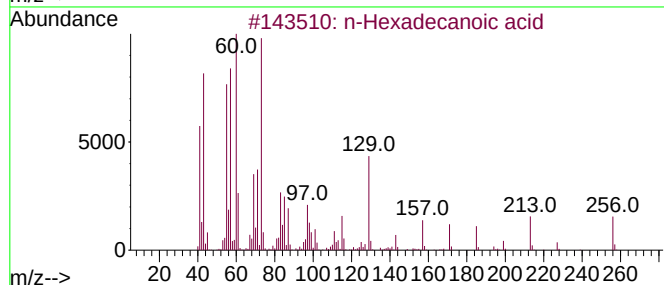
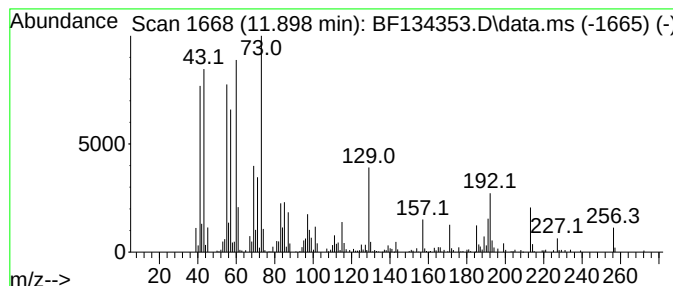
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.898	12.12 ng	259605	Phenanthrene-d10	11.369	
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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60



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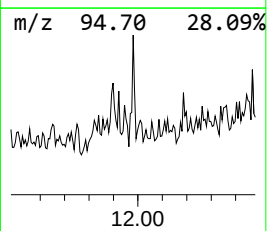
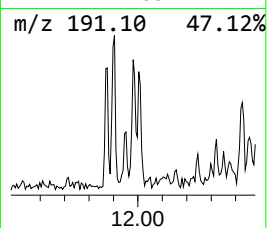
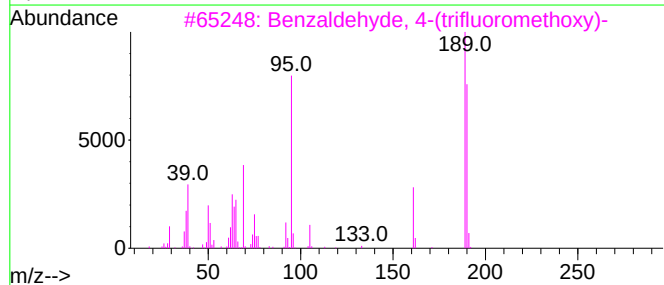
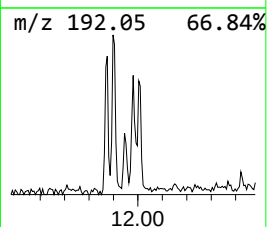
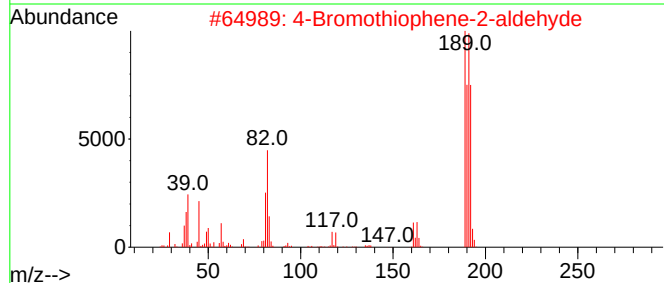
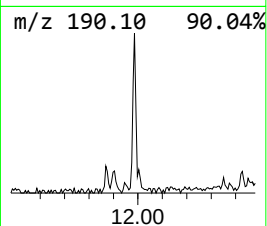
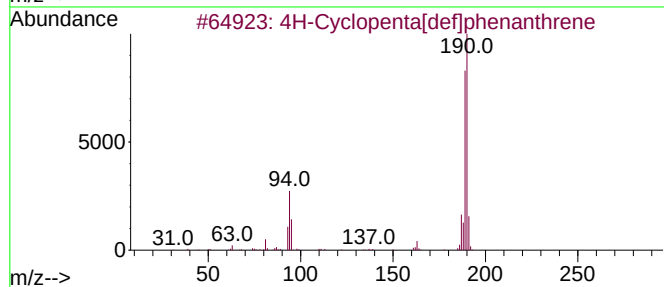
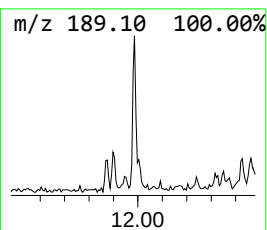
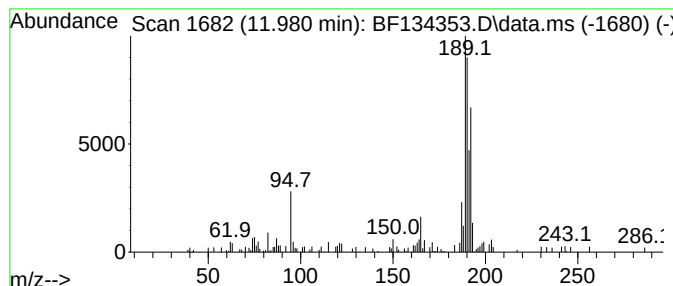
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ClientSampleId :
HR-1-071223

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.980	2.58 ng	55213	Phenanthrene-d10		11.369	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	52
2	4-Bromothiophene-2-aldehyde		190	C5H3BrOS	018791-75-8	50
3	Benzaldehyde, 4-(trifluoromethoxy)-		190	C8H5F3O2	000659-28-9	47
4	5H-Dibenzo[a,d]cycloheptene		192	C15H12	000256-81-5	35
5	Naphtho[2,3-b]norbornadiene		192	C15H12	107426-38-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134353.D
Acq On : 18 Jul 2023 23:34
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

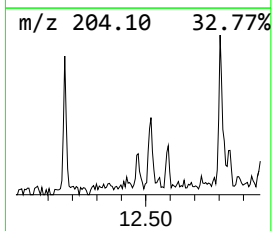
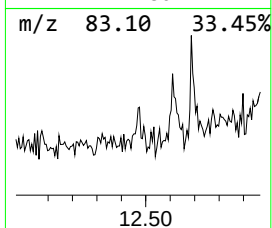
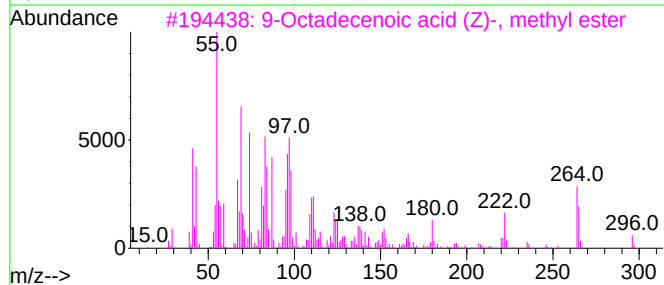
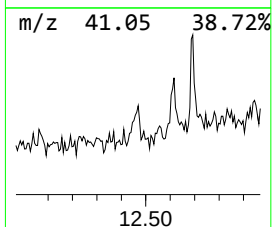
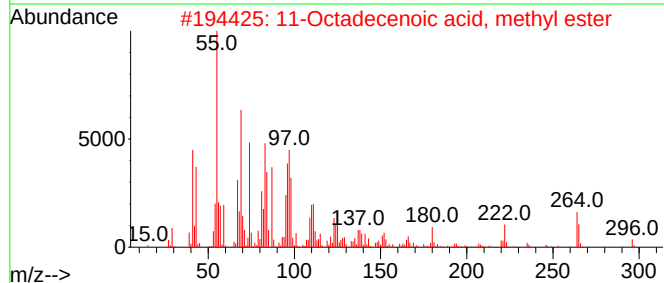
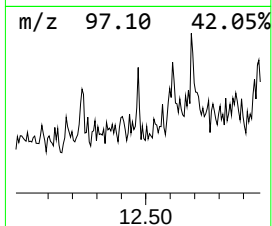
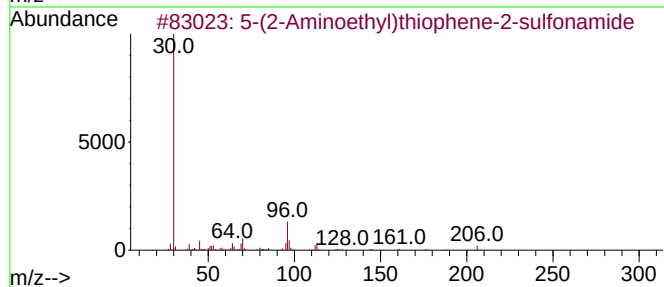
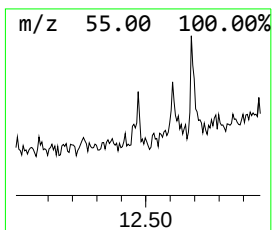
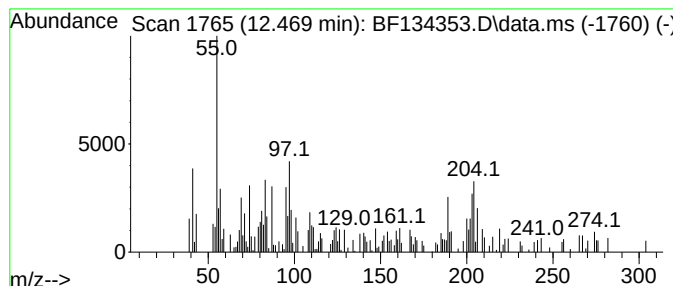
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ClientSampleId :
HR-1-071223

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.469 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.469	2.82 ng	60401	Phenanthrene-d10	11.369	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(2-Aminoethyl)thiophene-2-sulf...	206	C6H10N2O2S2	109213-13-0	35
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	18
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	14
4	1-Methylcyclohexylcarboxylic acid	142	C8H14O2	001123-25-7	14
5	Palmitoleic acid	254	C16H30O2	000373-49-9	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134353.D
Acq On : 18 Jul 2023 23:34
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

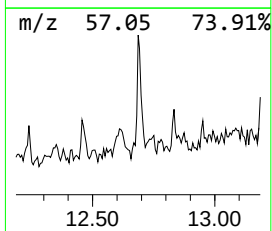
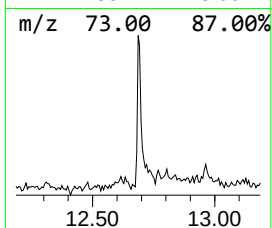
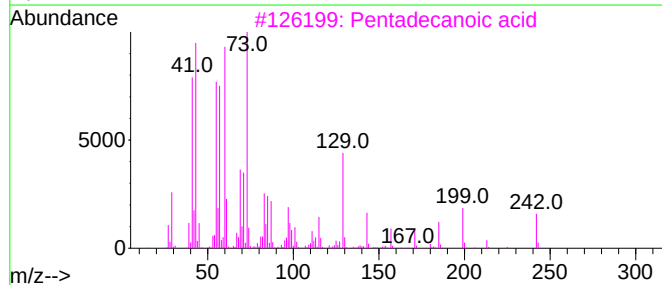
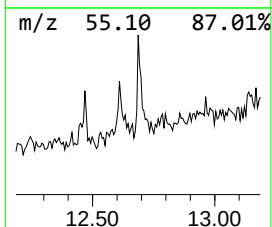
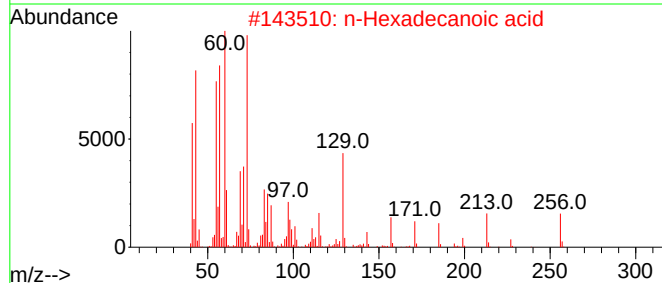
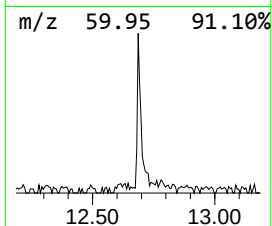
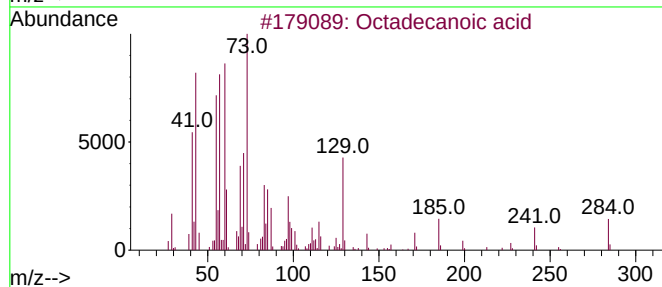
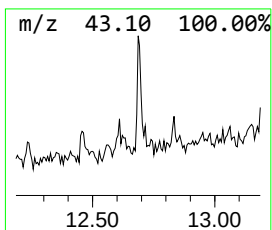
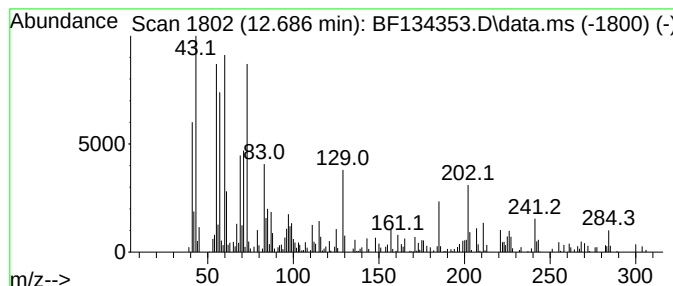
Instrument :
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ClientSampleId :
HR-1-071223

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.686	4.13 ng	88427	Phenanthrene-d10		11.369	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	62
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	62
4	Heptadecanoic acid		270	C17H34O2	000506-12-7	53
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134353.D
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Sample : 03601-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

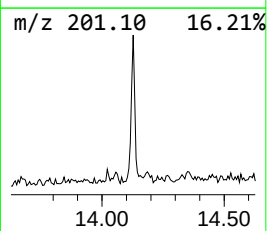
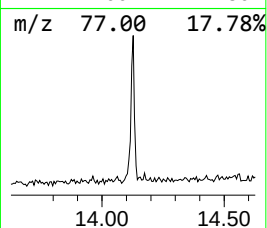
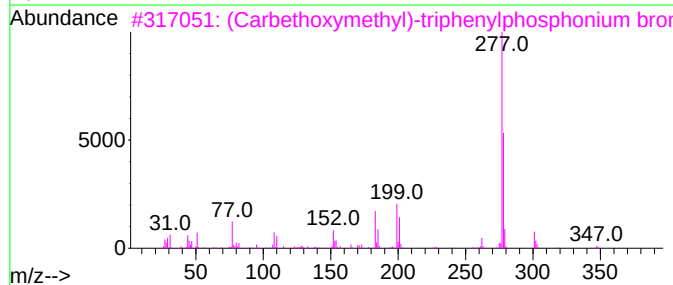
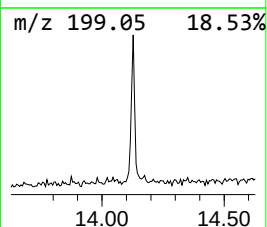
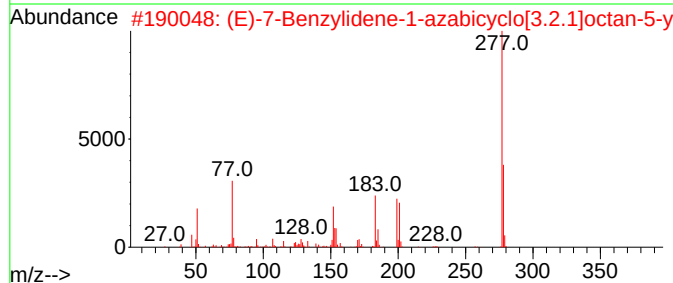
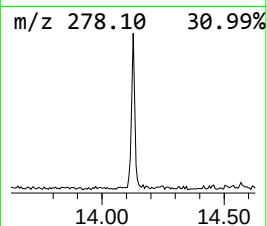
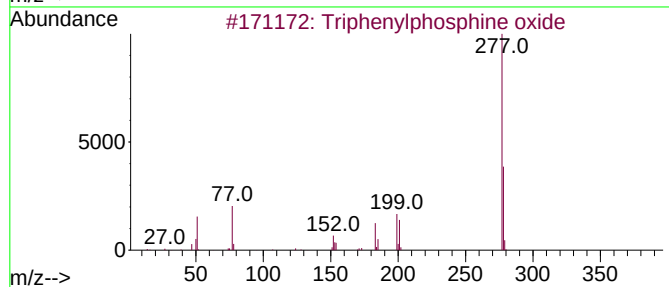
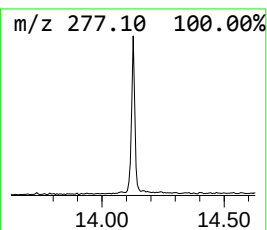
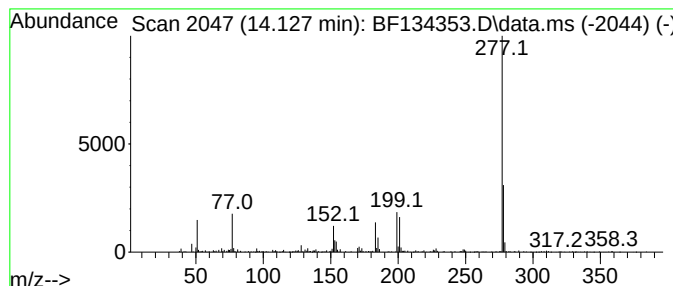
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.127	9.76 ng	230858	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	90
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	40
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	39
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134353.D
Acq On : 18 Jul 2023 23:34
Operator : CG\JU
Sample : 03601-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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
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Hexadecane, 2,6...	10.786	3.3	ng	70567	4	11.369	428406	20.0
unknown11.257	11.257	2.3	ng	49042	4	11.369	428406	20.0
n-Hexadecanoic ...	11.898	12.1	ng	259605	4	11.369	428406	20.0
4H-Cyclopenta[d...	11.980	2.6	ng	55213	4	11.369	428406	20.0
unknown12.469	12.469	2.8	ng	60401	4	11.369	428406	20.0
Octadecanoic acid	12.686	4.1	ng	88427	4	11.369	428406	20.0
Triphenylphosph...	14.127	9.8	ng	230858	5	14.033	472876	20.0