

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042321\
 Data File : BF123697.D
 Acq On : 23 Apr 2021 17:14
 Operator : JU/CG
 Sample : M2150-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-20

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-BF041521.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123697.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.440	567	570	576	rBV	2308541	2029692	27.39%	4.357%
2	6.457	739	743	754	rVB2	1624438	1850635	24.98%	3.973%
3	6.828	802	806	809	rBV	1878312	1451702	19.59%	3.116%
4	6.987	829	833	836	rBV	6282469	5425190	73.22%	11.646%
5	7.010	836	837	841	rVB	316769	178998	2.42%	0.384%
6	7.393	893	902	905	rBV	5058155	5115544	69.04%	10.982%
7	7.475	912	916	920	rBV5	61973	85134	1.15%	0.183%
8	7.551	927	929	933	rVB2	118028	103021	1.39%	0.221%
9	7.851	973	980	985	rBV4	186013	288091	3.89%	0.618%
10	8.116	1020	1025	1027	rBV	2100589	1924066	25.97%	4.130%
11	8.134	1027	1028	1031	rVV	720053	459516	6.20%	0.986%
12	8.187	1034	1037	1039	rVB	106535	89367	1.21%	0.192%
13	8.457	1074	1083	1087	rBV4	60884	87422	1.18%	0.188%
14	8.828	1143	1146	1149	rVB	680702	497740	6.72%	1.069%
15	8.928	1158	1163	1166	rVB	359033	298293	4.03%	0.640%
16	9.028	1172	1180	1185	rBV	33876	93441	1.26%	0.201%
17	9.198	1203	1209	1212	rBV	7735857	7409177	100.00%	15.906%
18	9.586	1272	1275	1278	rBV	287733	212140	2.86%	0.455%
19	9.734	1294	1300	1310	rVB8	61580	136876	1.85%	0.294%
20	9.875	1317	1324	1327	rBV	2138404	1833228	24.74%	3.935%
21	9.904	1327	1329	1332	rVB	376109	274324	3.70%	0.589%
22	10.075	1355	1358	1363	rBV	251439	238638	3.22%	0.512%
23	10.422	1414	1417	1424	rVB	230188	216067	2.92%	0.464%
24	10.510	1424	1432	1434	rBV8	44002	97440	1.32%	0.209%
25	10.663	1453	1458	1461	rBV	3849207	3245564	43.80%	6.967%
26	11.233	1548	1555	1557	rBV4	55177	97081	1.31%	0.208%
27	11.363	1573	1577	1579	rBV	2023720	1708764	23.06%	3.668%
28	11.380	1579	1580	1583	rVB	228348	175739	2.37%	0.377%
29	11.586	1611	1615	1618	rBV2	103437	124823	1.68%	0.268%
30	11.657	1624	1627	1630	rBV3	85091	82735	1.12%	0.178%
31	11.898	1663	1668	1674	rBV	843255	826145	11.15%	1.774%
32	12.280	1730	1733	1737	rVB	90172	81894	1.11%	0.176%
33	12.345	1741	1744	1749	rVB	127931	113593	1.53%	0.244%
34	12.686	1799	1802	1809	rBV	210684	218310	2.95%	0.469%
35	12.957	1843	1848	1851	rBV	6820186	6019716	81.25%	12.923%
36	13.498	1936	1940	1944	rBV2	90618	137878	1.86%	0.296%

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37	13.898	2003	2008	2022	rVB6	153931	474557	6.40%	1.019%
38	14.010	2023	2027	2030	rVB	1286874	1181318	15.94%	2.536%
39	14.486	2105	2108	2113	rBV	90222	80964	1.09%	0.174%
40	14.792	2158	2160	2165	rVB	91781	98486	1.33%	0.211%
41	15.139	2215	2219	2222	rVB	89559	102565	1.38%	0.220%
42	15.480	2272	2277	2281	rBV	988944	1195307	16.13%	2.566%
43	15.521	2281	2284	2288	rVB	96079	110518	1.49%	0.237%
44	15.957	2354	2358	2366	rVB	72856	110532	1.49%	0.237%

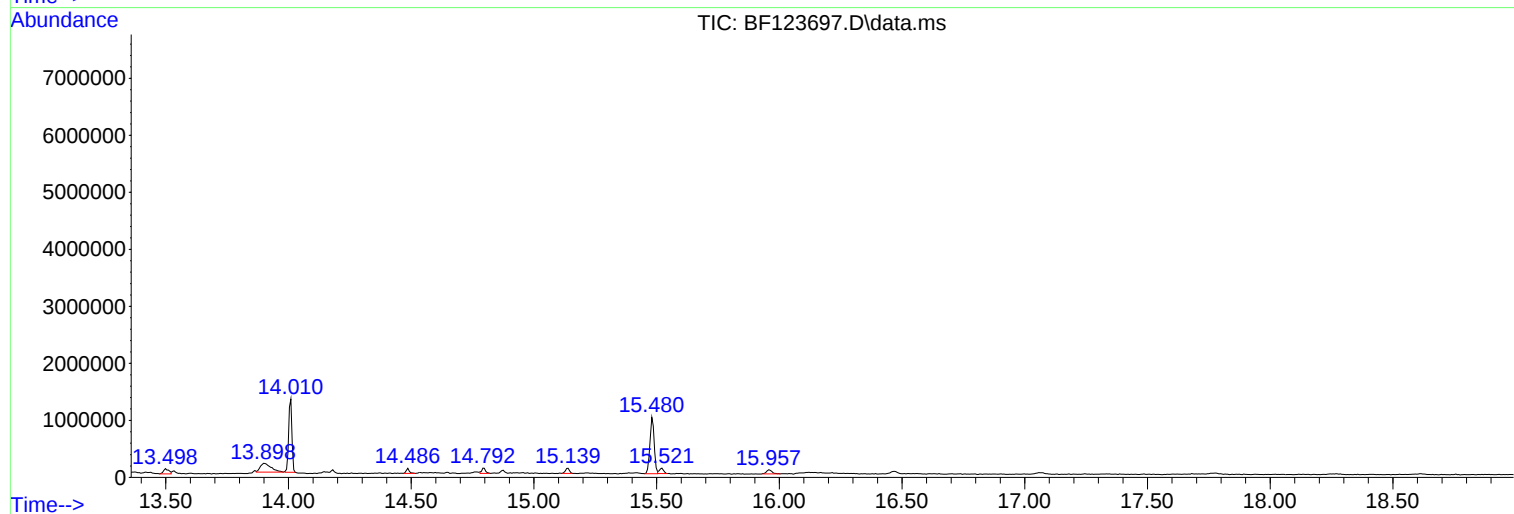
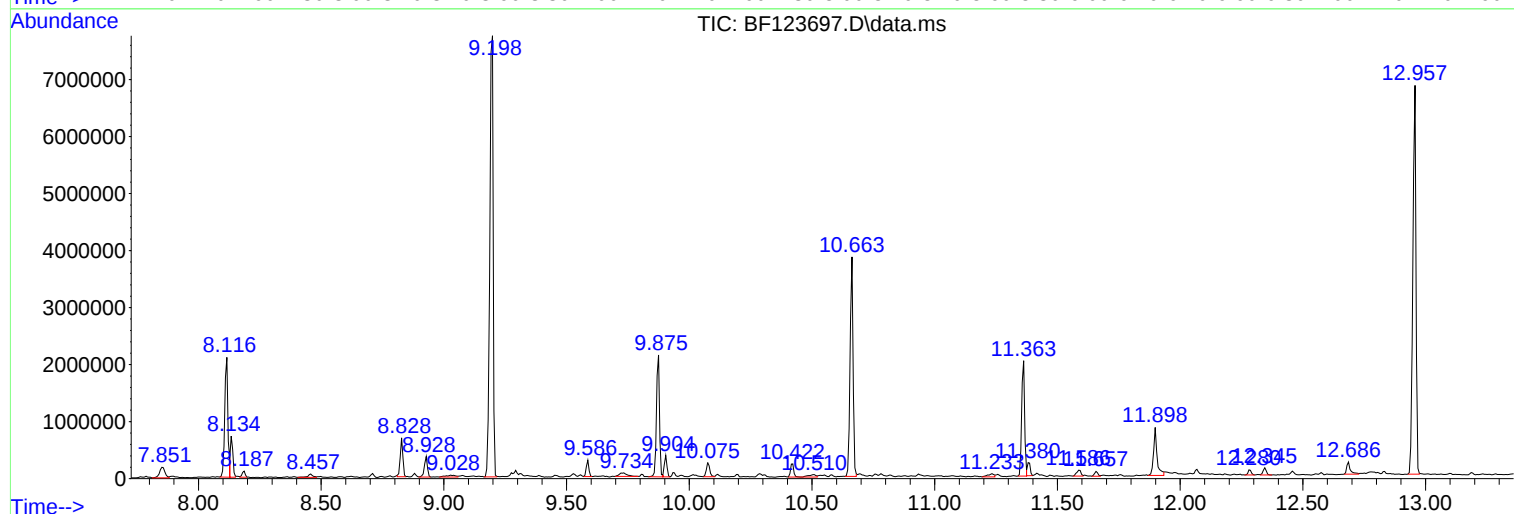
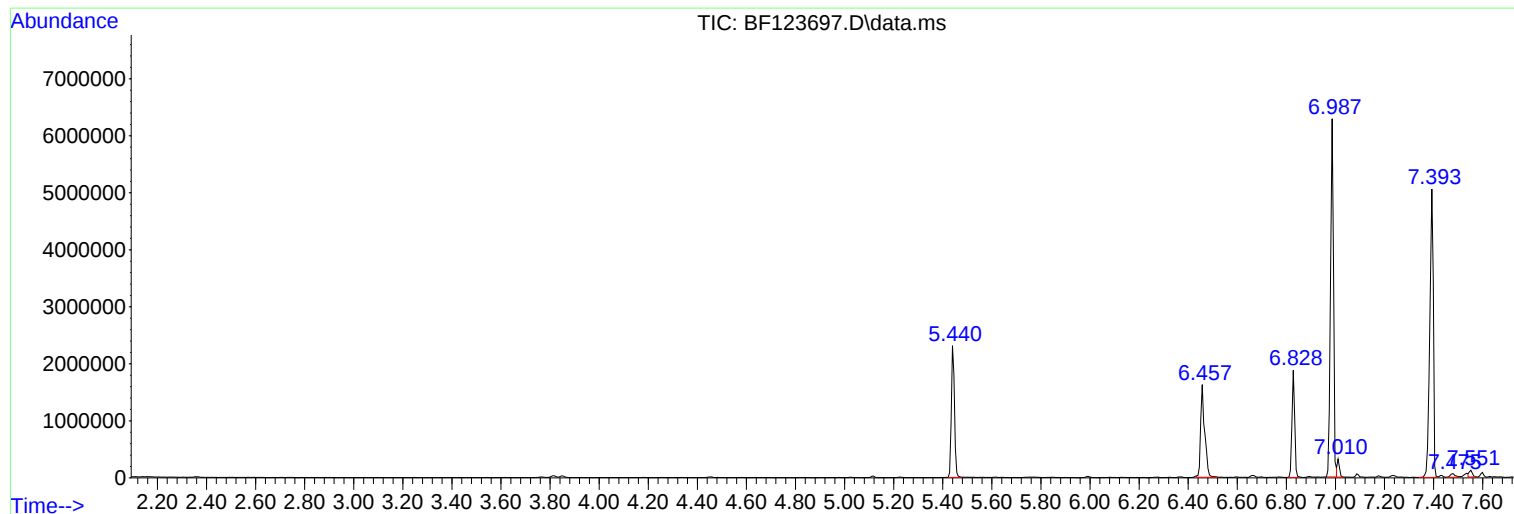
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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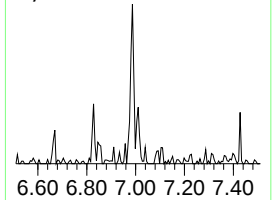
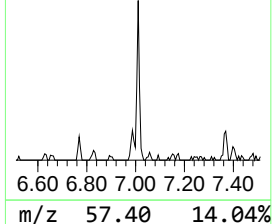
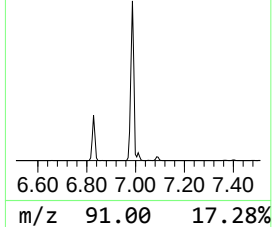
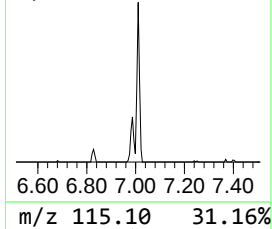
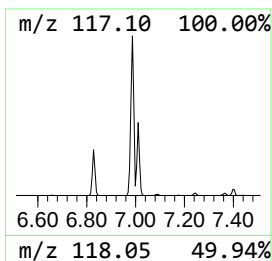
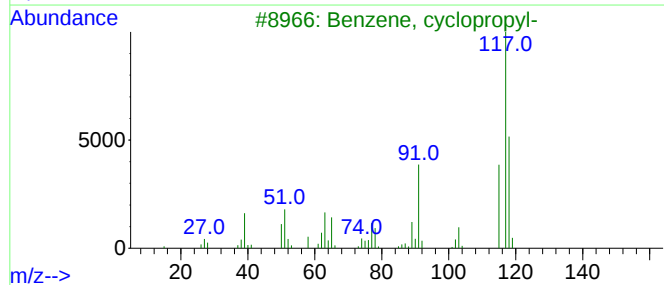
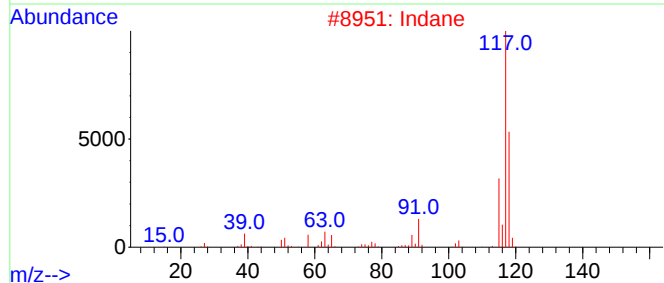
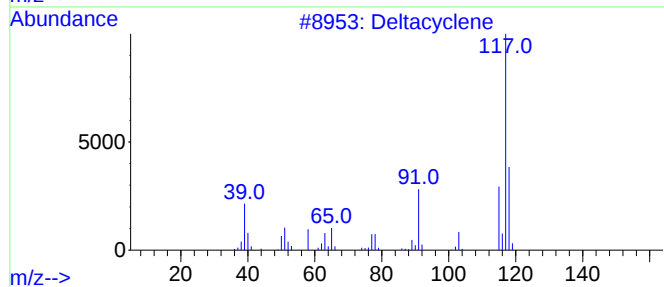
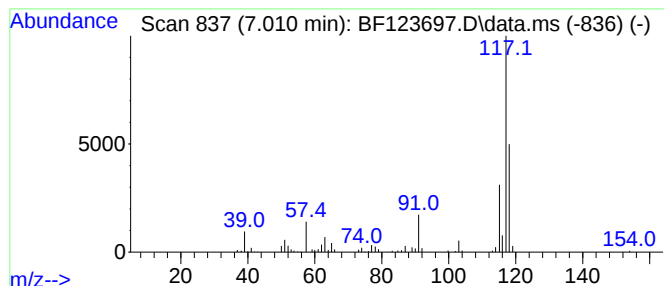
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Deltacyclene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.010	2.47 ng	178998	1,4-Dichlorobenzene-d4	6.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Deltacyclene	118	C9H10	007785-10-6	81
2		Indane	118	C9H10	000496-11-7	72
3		Benzene, cyclopropyl-	118	C9H10	000873-49-4	59
4		Benzene, 2-propenyl-	118	C9H10	000300-57-2	46
5		Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	46



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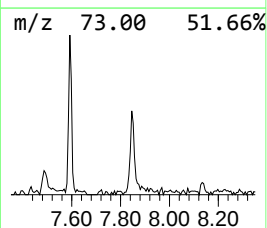
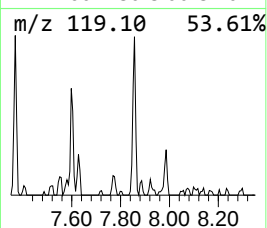
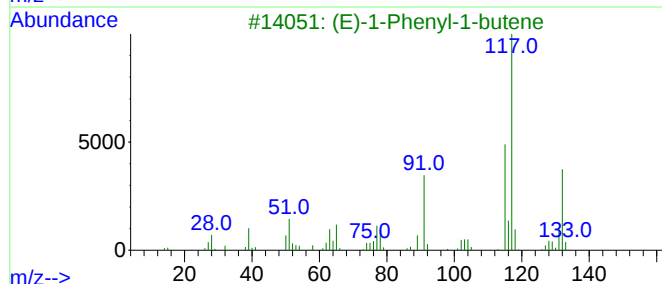
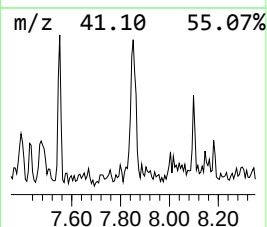
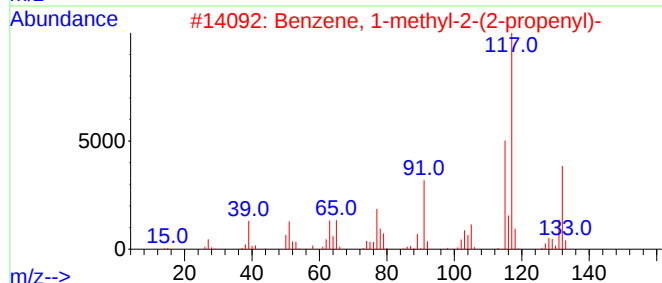
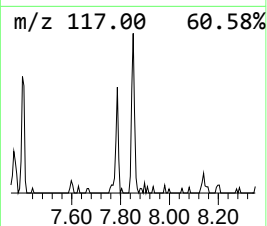
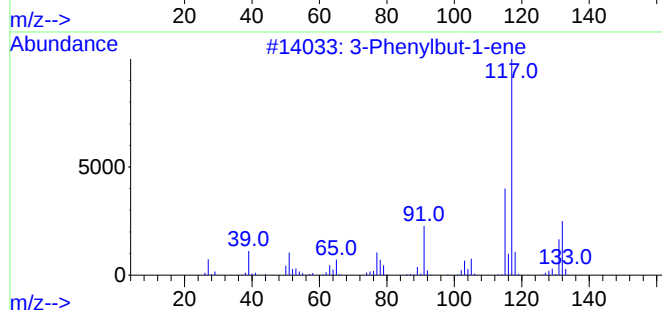
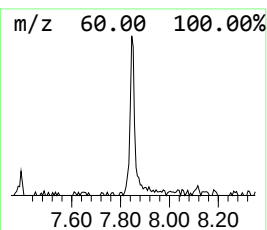
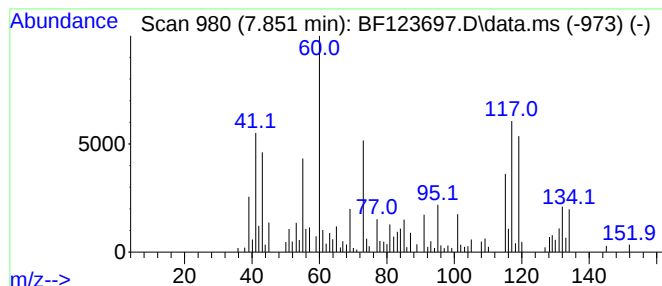
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.85 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.851	2.99 ng	288091	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Phenylbut-1-ene	132	C10H12	000934-10-1	30
2			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	30
3			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	25
4			Indan, 1-methyl-	132	C10H12	000767-58-8	18
5			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	18



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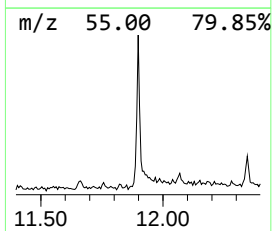
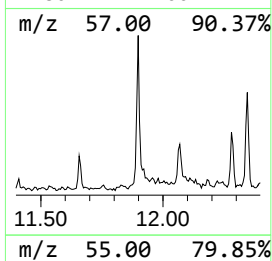
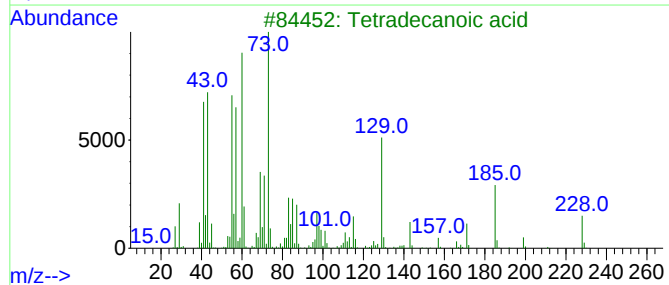
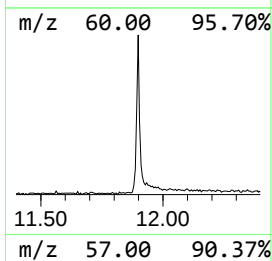
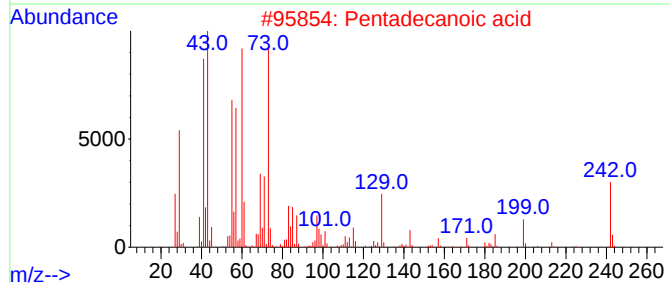
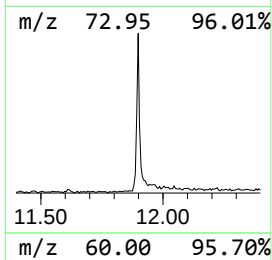
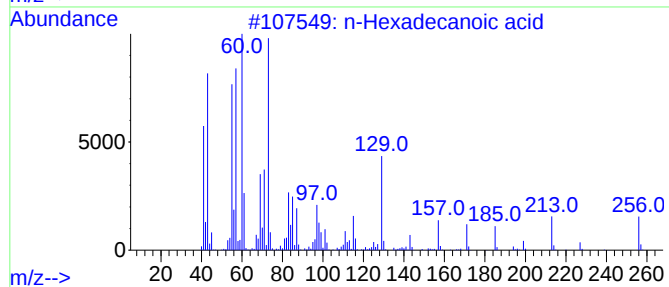
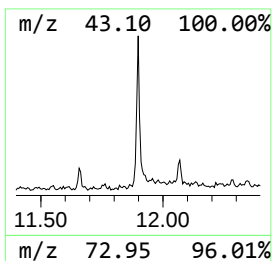
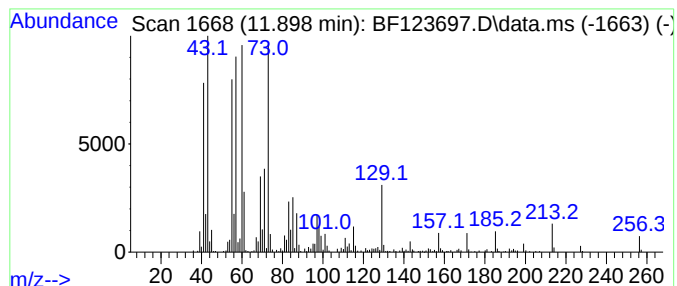
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	9.67 ng	826145	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	87
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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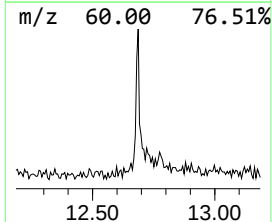
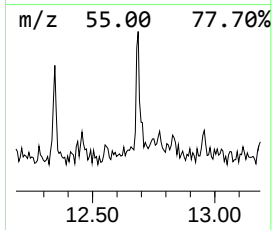
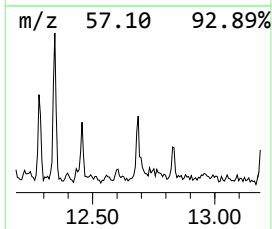
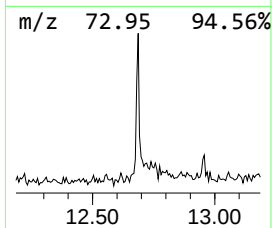
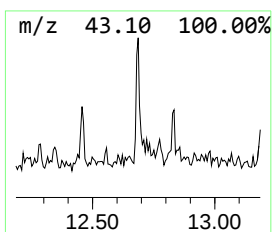
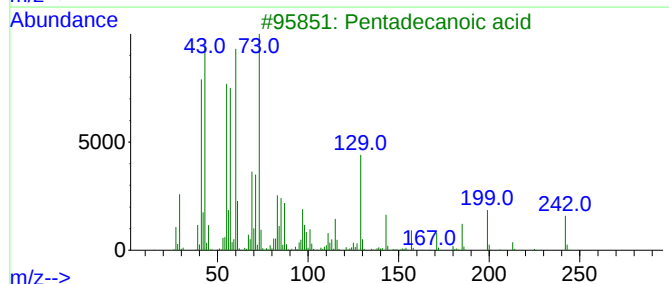
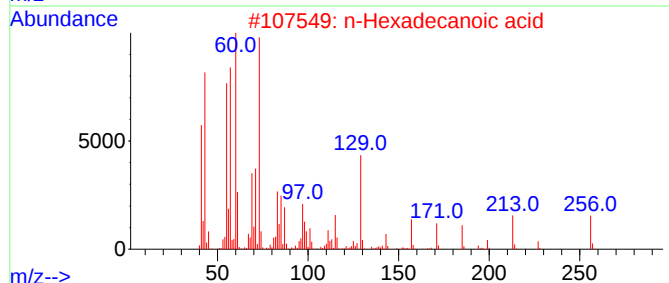
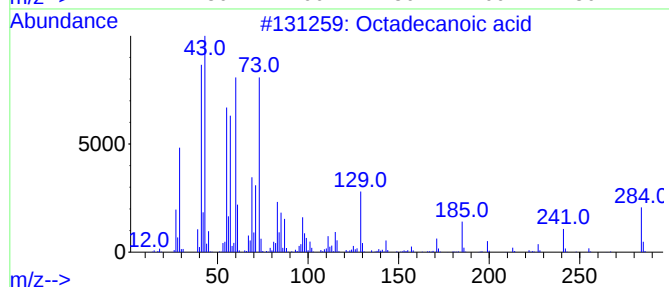
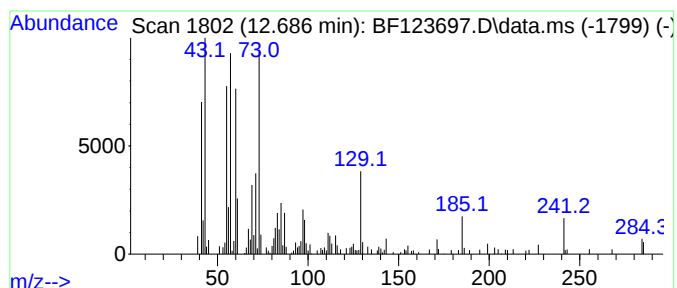
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	3.70 ng	218310	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64



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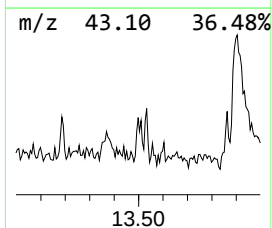
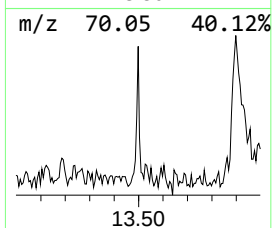
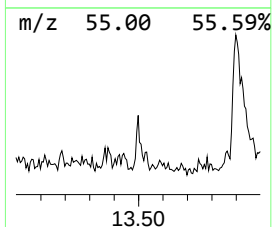
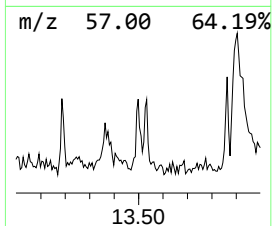
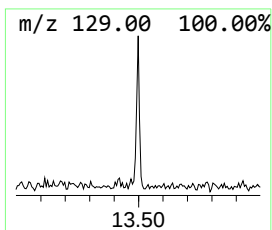
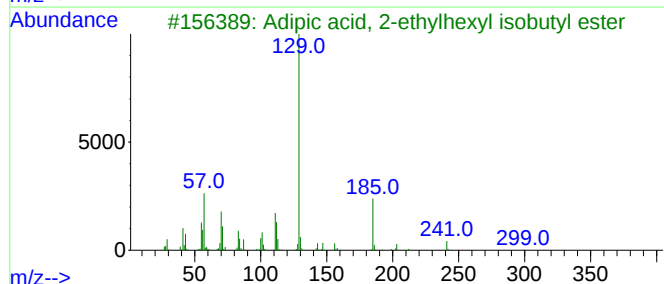
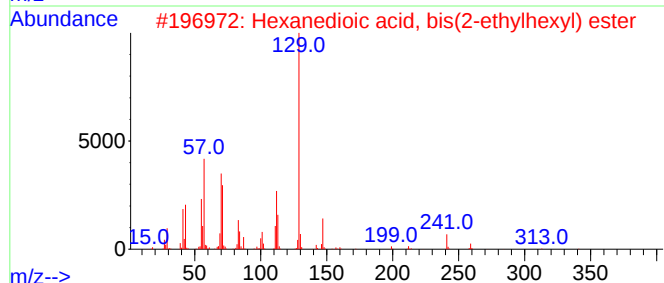
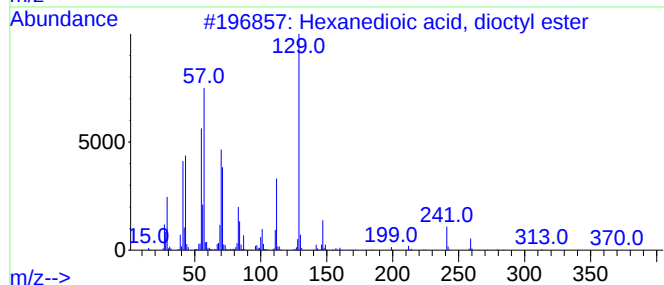
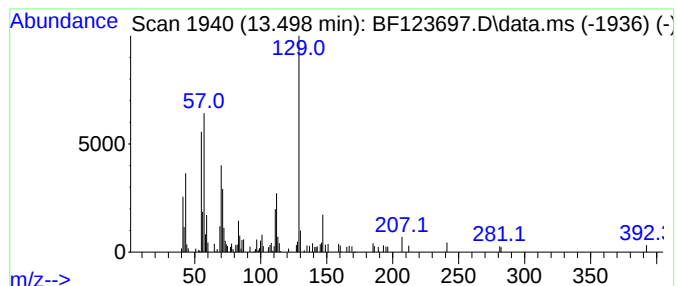
Instrument :
BNA_F
ClientSampled :
TWP-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexanedioic acid, dioctyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.498	2.33 ng	137878	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	83
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	80
3	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	52
4	Adipic acid, octyl 3-pentyl ester	328	C19H36O4	1000324-61-0	43
5	Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042321\
Data File : BF123697.D
Acq On : 23 Apr 2021 17:14
Operator : JU/CG
Sample : M2150-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

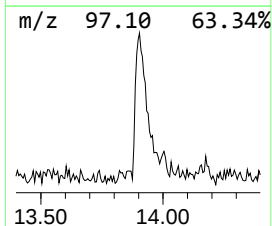
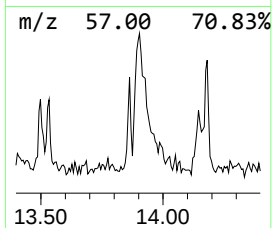
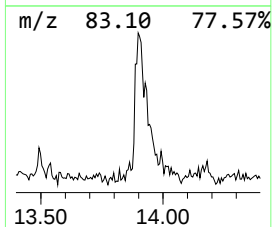
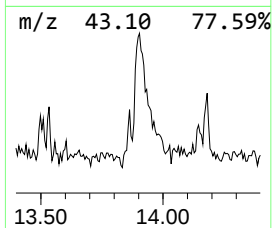
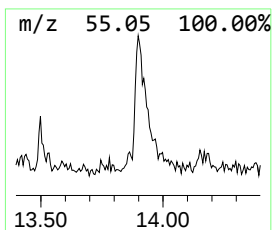
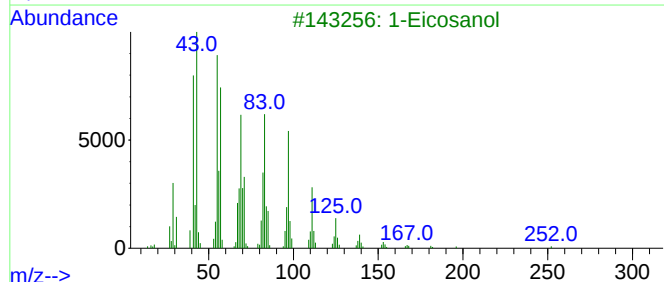
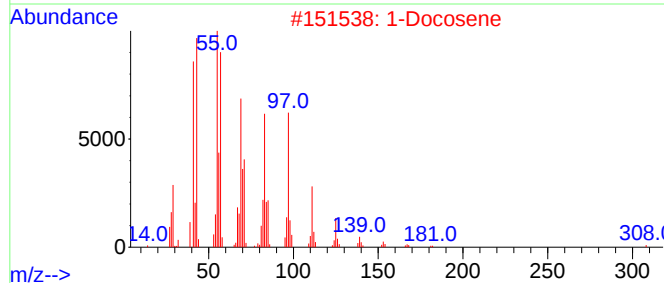
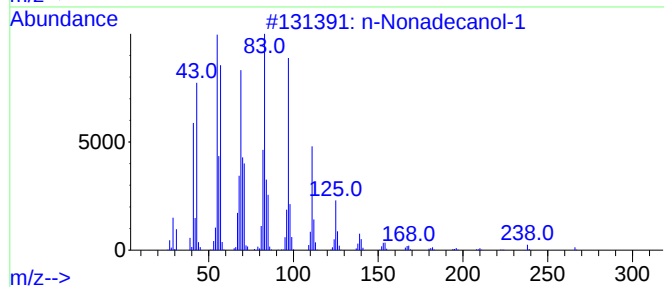
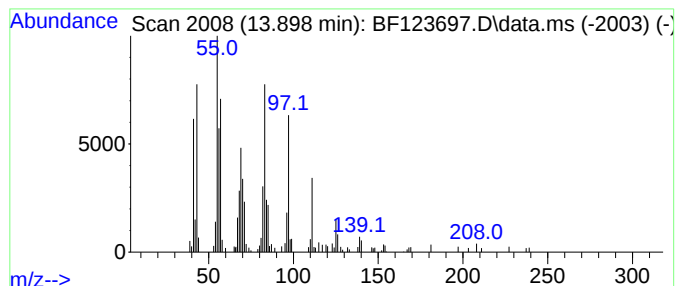
Instrument :
BNA_F
ClientSampleId :
TWP-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.898	8.03 ng	474557	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
2	1-Docosene	308	C22H44	001599-67-3	90
3	1-Eicosanol	298	C20H42O	000629-96-9	86
4	17-Pentatriacontene	491	C35H70	006971-40-0	86
5	1-Heneicosanol	312	C21H44O	015594-90-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042321\
Data File : BF123697.D
Acq On : 23 Apr 2021 17:14
Operator : JU/CG
Sample : M2150-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Deltacyclene	7.010	2.5	ng	178998	1	6.828	1451700	20.0
unknown7.85	7.851	3.0	ng	288091	2	8.116	1924070	20.0
n-Hexadecanoic ...	11.898	9.7	ng	826145	4	11.363	1708760	20.0
Octadecanoic acid	12.686	3.7	ng	218310	5	14.010	1181320	20.0
Hexanedioic aci...	13.498	2.3	ng	137878	5	14.010	1181320	20.0
n-Nonadecanol-1	13.898	8.0	ng	474557	5	14.010	1181320	20.0