

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
 Data File : BF133641.D
 Acq On : 08 Jun 2023 14:31
 Operator : CG\JU
 Sample : 03049-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-01-060523

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133641.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.892	302	307	314	rVB	151117	200334	9.85%	1.184%
2	4.187	354	357	365	rBV	21356	34393	1.69%	0.203%
3	4.345	382	384	392	rBV	22611	35959	1.77%	0.213%
4	4.992	478	494	497	rBV	269241	1038413	51.07%	6.138%
5	5.051	500	504	512	rVB	28729	44478	2.19%	0.263%
6	5.457	568	573	576	rBV	1820162	1719125	84.55%	10.161%
7	6.463	739	744	747	rBV	1892210	1749793	86.06%	10.343%
8	6.757	791	794	801	rBV	36664	32683	1.61%	0.193%
9	6.833	804	807	811	rBV	962759	813695	40.02%	4.810%
10	7.398	899	903	906	rBV	1402986	1096726	53.94%	6.483%
11	7.739	958	961	963	rBV	33866	25435	1.25%	0.150%
12	7.763	963	965	968	rVB	34850	27980	1.38%	0.165%
13	7.922	990	992	1000	rVB	20016	24921	1.23%	0.147%
14	8.122	1022	1026	1028	rBV	1238517	1008301	49.59%	5.960%
15	8.139	1028	1029	1041	rVB	59045	50499	2.48%	0.298%
16	8.698	1121	1124	1130	rBV	26614	34300	1.69%	0.203%
17	9.198	1205	1209	1212	rBV	2362016	2033339	100.00%	12.019%
18	9.733	1297	1300	1303	rBV	32273	27711	1.36%	0.164%
19	9.874	1321	1324	1328	rBV	1293669	1033125	50.81%	6.107%
20	10.074	1354	1358	1364	rBV3	30016	35784	1.76%	0.212%
21	10.304	1394	1397	1400	rVB	38956	30402	1.50%	0.180%
22	10.421	1413	1417	1422	rBV	22142	23798	1.17%	0.141%
23	10.527	1430	1435	1439	rBV	17093	23626	1.16%	0.140%
24	10.586	1442	1445	1448	rBV	134300	120456	5.92%	0.712%
25	10.663	1454	1458	1462	rBV	1233044	1045147	51.40%	6.178%
26	10.792	1475	1480	1484	rVB2	32882	47033	2.31%	0.278%
27	11.227	1551	1554	1557	rBV	43069	38186	1.88%	0.226%
28	11.257	1557	1559	1565	rVB	24981	28785	1.42%	0.170%
29	11.363	1574	1577	1580	rBV	1067071	937400	46.10%	5.541%
30	11.386	1580	1581	1584	rVV	72784	49949	2.46%	0.295%
31	11.439	1588	1590	1593	rVB	30998	24349	1.20%	0.144%
32	11.892	1664	1667	1672	rBV2	138412	126692	6.23%	0.749%
33	12.063	1694	1696	1699	rBV	34115	32131	1.58%	0.190%
34	12.457	1760	1763	1768	rVB2	44416	51470	2.53%	0.304%
35	12.580	1781	1784	1787	rBV	105490	91123	4.48%	0.539%
36	12.674	1798	1800	1803	rBV4	23634	25154	1.24%	0.149%

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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-BF052523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.810	1820	1823	1825	rBV	96204	80198	3.94%	0.474%
38	12.957	1844	1848	1851	rBV	1630133	1540055	75.74%	9.103%
39	13.857	1998	2001	2008	rBV	181359	258889	12.73%	1.530%
40	14.009	2023	2027	2030	rBV	785392	736580	36.23%	4.354%
41	15.133	2215	2218	2220	rBV	80634	81938	4.03%	0.484%
42	15.480	2273	2277	2280	rBV	393438	457896	22.52%	2.707%

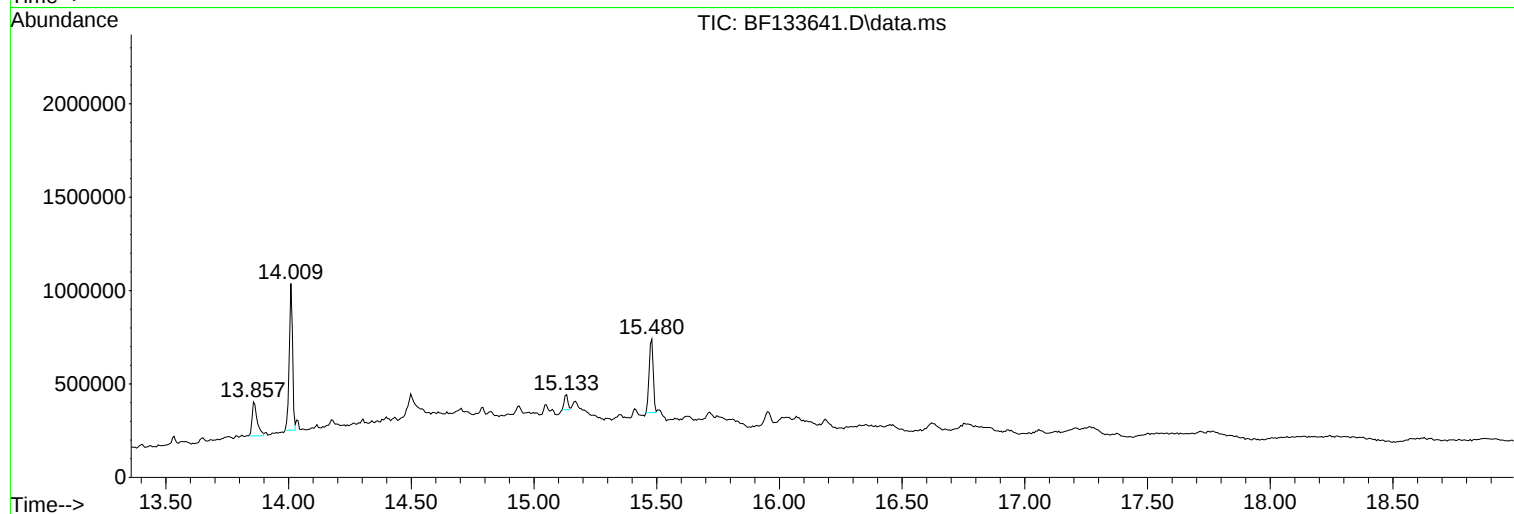
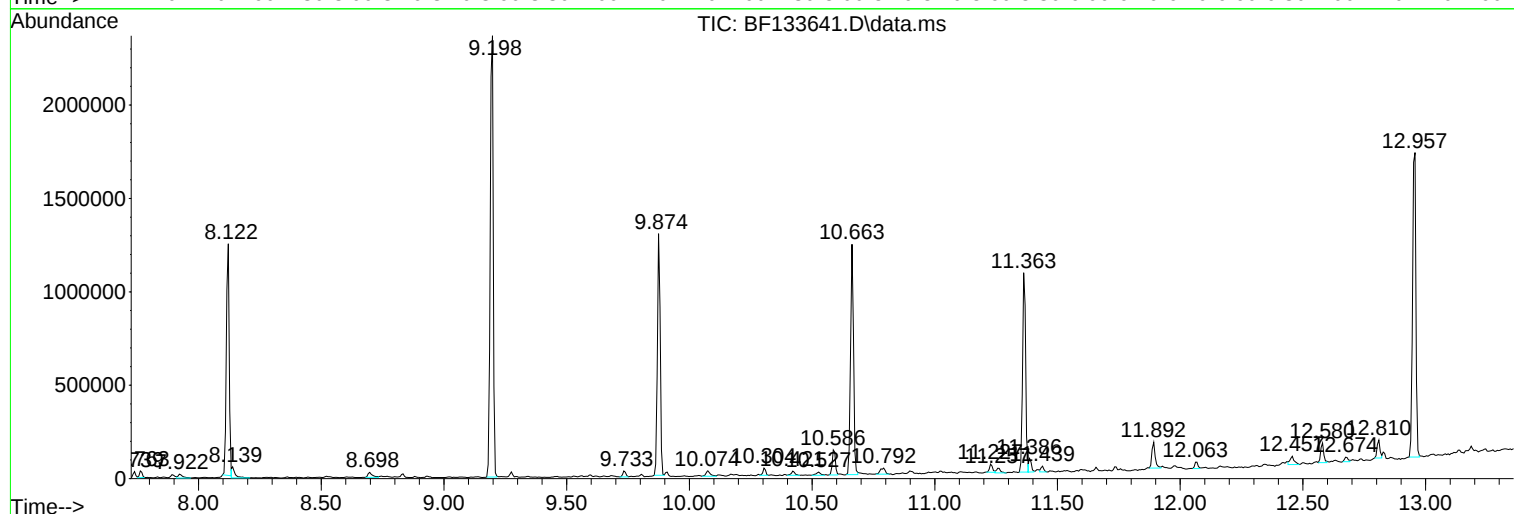
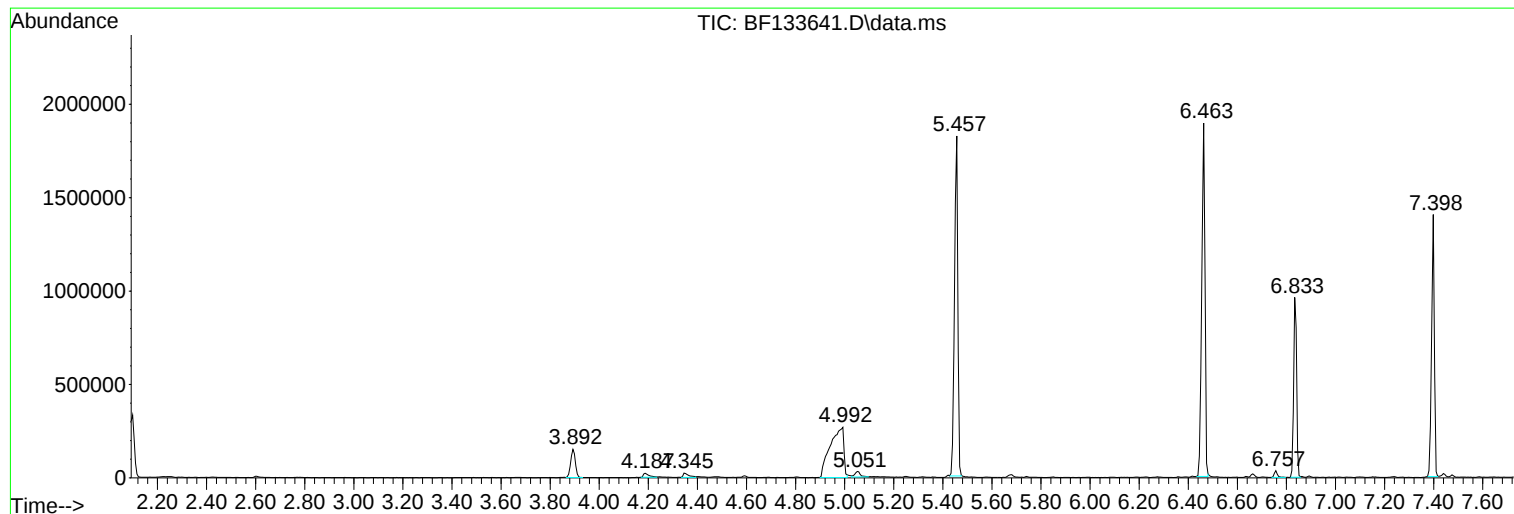
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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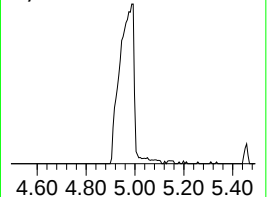
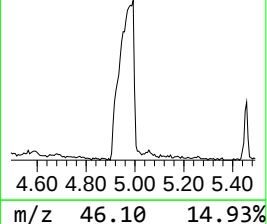
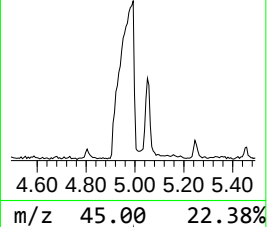
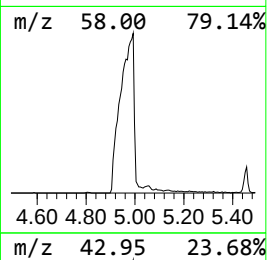
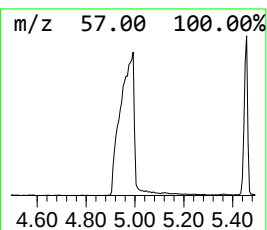
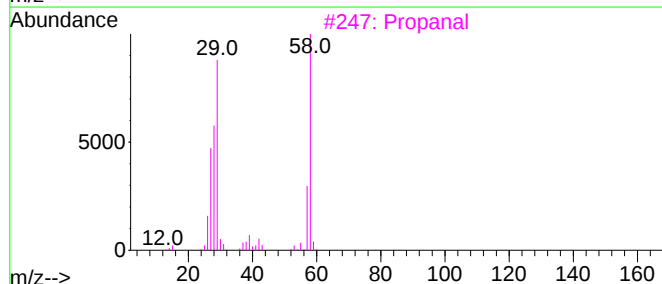
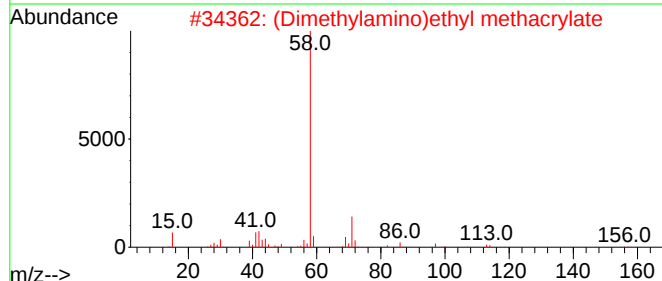
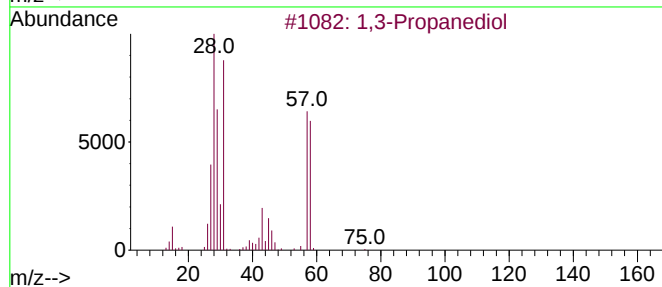
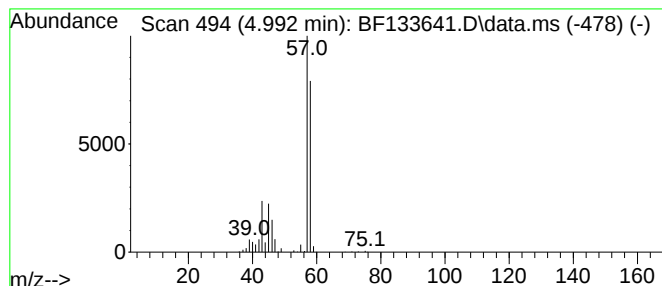
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown4.992 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.992	25.52 ng	1038410	1,4-Dichlorobenzene-d4	6.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Propanediol	76	C3H8O2	000504-63-2	43
2			(Dimethylamino)ethyl methacrylate	157	C8H15NO2	002867-47-2	28
3			Propanal	58	C3H6O	000123-38-6	9
4			Cyclopropyl methyl carbinol	86	C5H10O	000765-42-4	9
5			Formic acid, 2-propenyl ester	86	C4H6O2	001838-59-1	9



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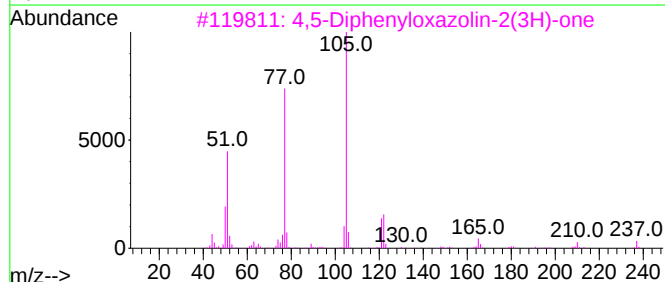
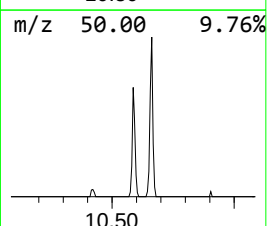
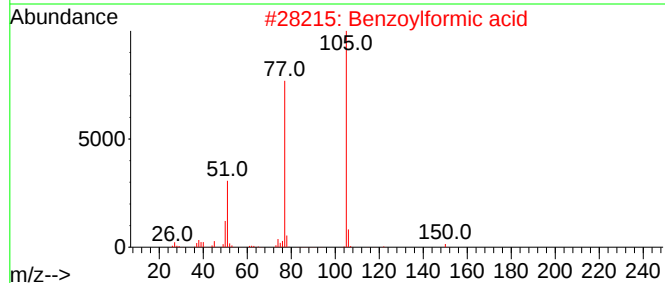
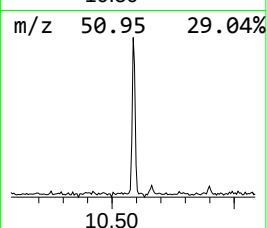
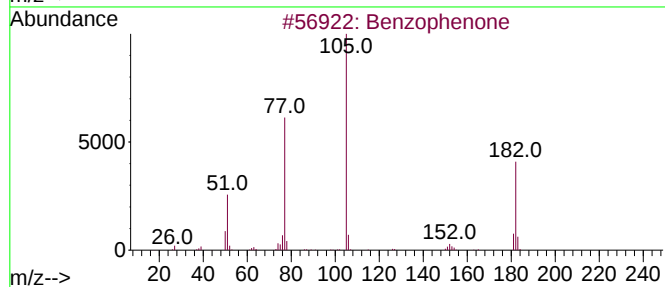
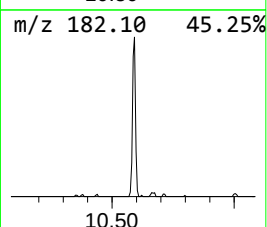
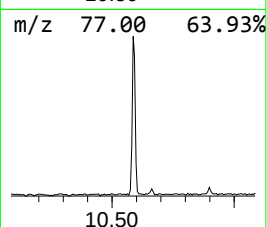
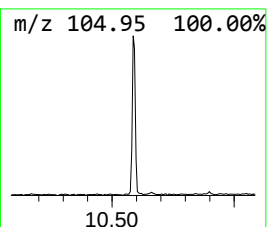
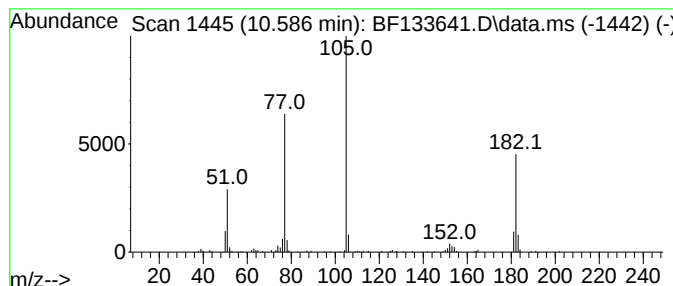
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	2.33 ng	120456	Acenaphthene-d10	9.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzoylformic acid	150	C8H6O3	000611-73-4	49
3			4,5-Diphenyloxazolin-2(3H)-one	237	C15H11NO2	005014-83-5	47
4			Benzilamide	227	C14H13NO2	004746-87-6	47
5			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47



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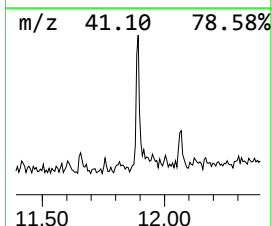
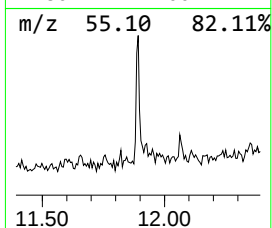
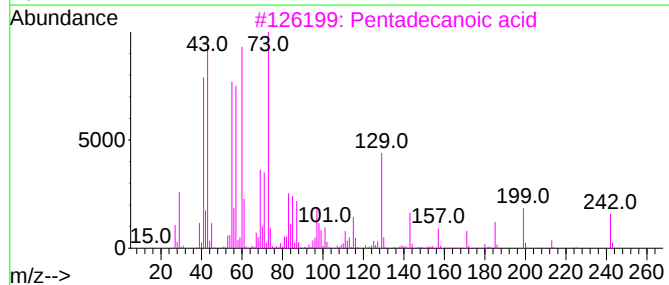
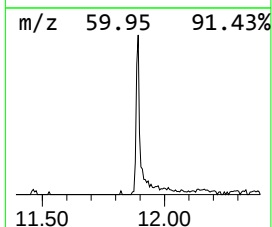
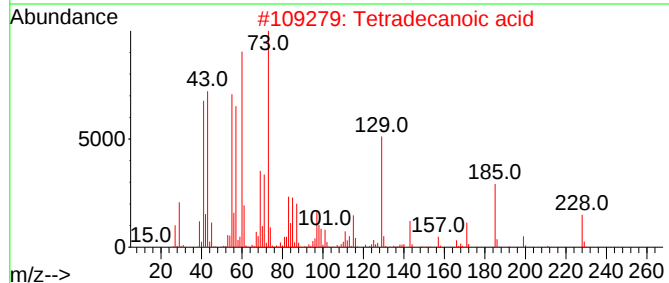
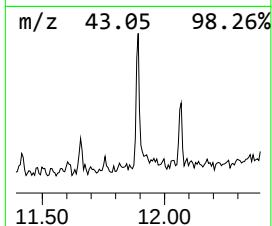
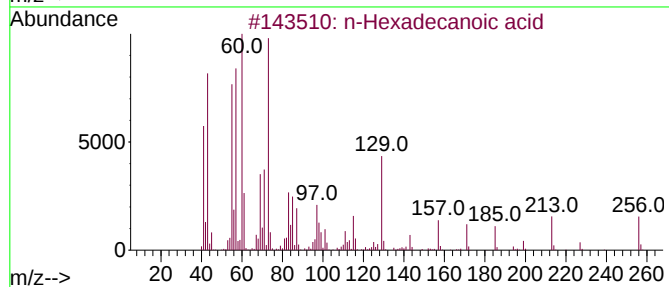
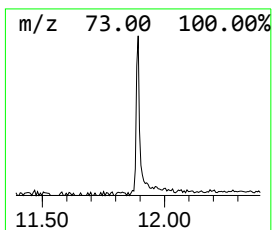
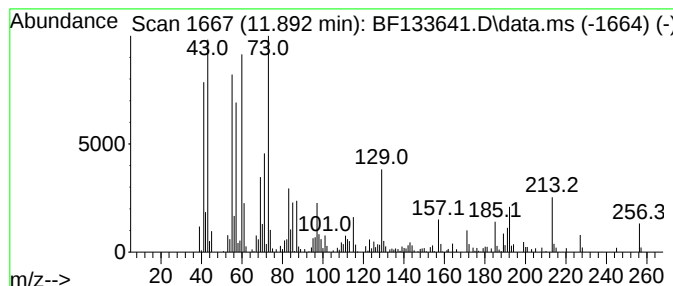
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	2.70 ng	126692	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	62
5			n-Decanoic acid	172	C10H20O2	000334-48-5	55



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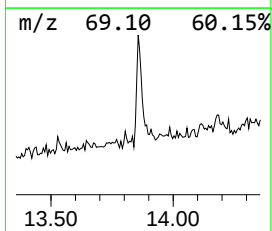
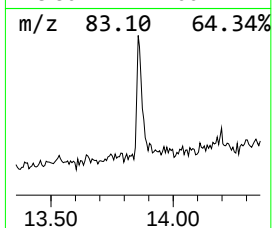
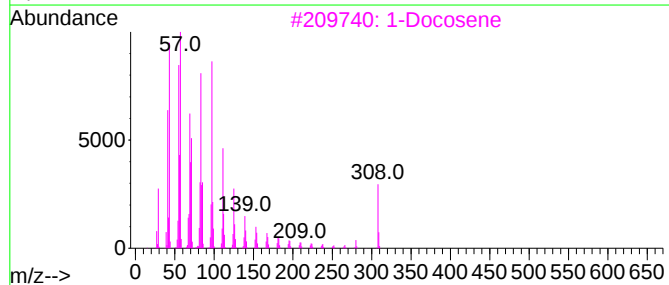
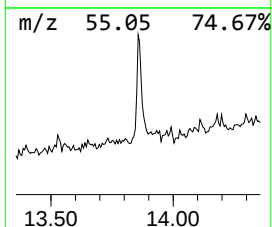
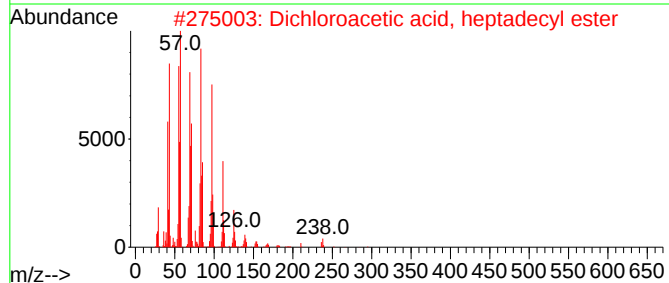
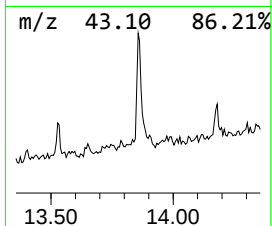
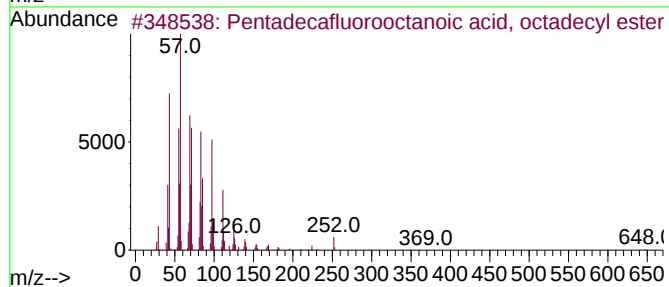
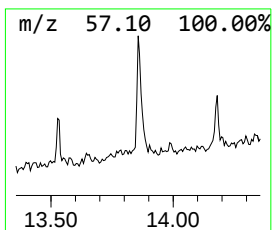
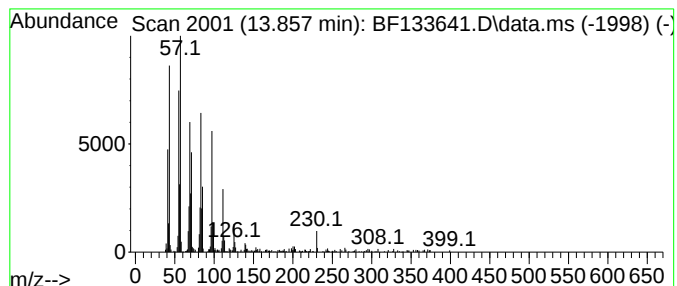
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.857	7.03 ng	258889	Chrysene-d12	14.009	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3	1-Docosene	308	C22H44	001599-67-3	93
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91



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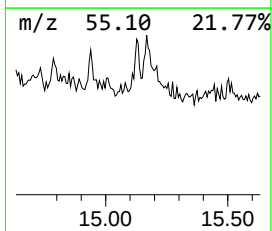
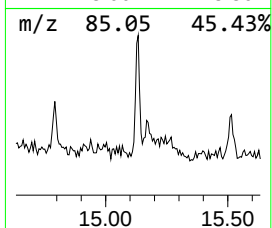
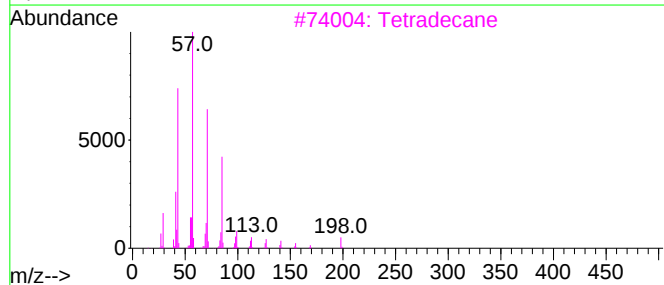
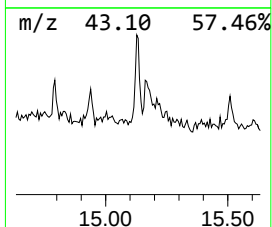
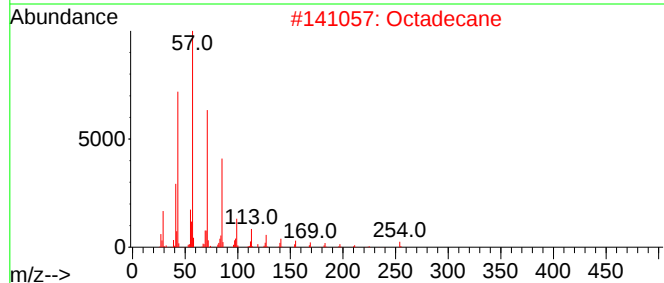
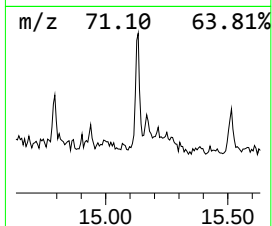
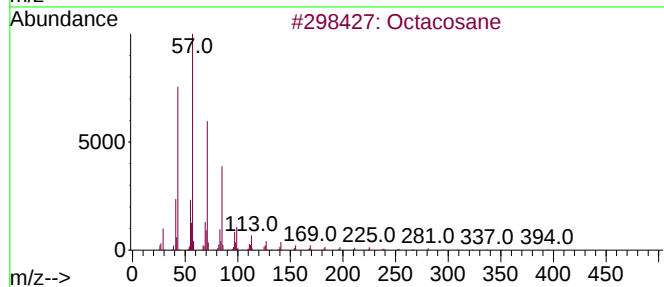
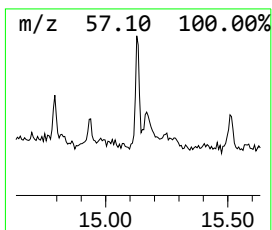
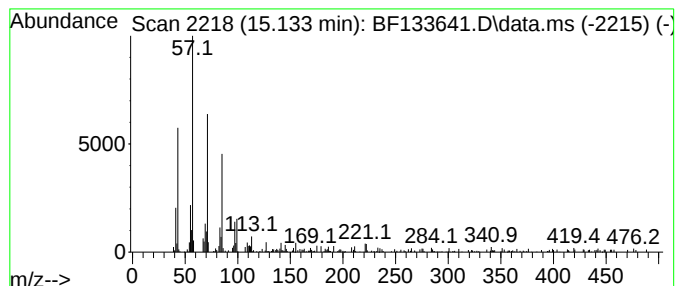
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	3.58 ng	81938	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	96
2			Octadecane	254	C18H38	000593-45-3	93
3			Tetradecane	198	C14H30	000629-59-4	81
4			Hexacosane	366	C26H54	000630-01-3	81
5			Docosane	310	C22H46	000629-97-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133641.D
Acq On : 08 Jun 2023 14:31
Operator : CG\JU
Sample : 03049-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-01-060523

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown4.992	4.992	25.5	ng	1038410	1	6.833	813695	20.0
Benzophenone	10.586	2.3	ng	120456	3	9.874	1033130	20.0
n-Hexadecanoic ...	11.892	2.7	ng	126692	4	11.363	937400	20.0
Pentadecafluoro...	13.857	7.0	ng	258889	5	14.009	736580	20.0
Octacosane	15.133	3.6	ng	81938	6	15.480	457896	20.0