

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
 Data File : BF133780.D
 Acq On : 15 Jun 2023 17:55
 Operator : CG\JU
 Sample : 03140-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3-GA

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133780.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.881	301	305	311	rVB	47333	66041	3.02%	0.408%
2	5.045	499	503	512	rVB	48158	63232	2.89%	0.390%
3	5.416	562	566	567	rBV	40255	34008	1.56%	0.210%
4	5.445	567	571	574	rVB	2247342	2119803	96.94%	13.088%
5	6.457	739	743	746	rBV	2000576	2099536	96.01%	12.962%
6	6.828	803	806	810	rBV	696155	600608	27.47%	3.708%
7	7.392	898	902	905	rBV	1555736	1323631	60.53%	8.172%
8	8.110	1021	1024	1027	rBV	775780	698642	31.95%	4.313%
9	8.133	1027	1028	1035	rVB	73335	47497	2.17%	0.293%
10	9.186	1203	1207	1211	rBV	2403455	2186686	100.00%	13.501%
11	9.869	1319	1323	1326	rBV	755549	591048	27.03%	3.649%
12	10.580	1440	1444	1448	rBV	116063	92856	4.25%	0.573%
13	10.657	1453	1457	1467	rBV	1505902	1290128	59.00%	7.965%
14	10.892	1494	1497	1502	rVB	27691	24950	1.14%	0.154%
15	11.357	1572	1576	1579	rBV	760069	645165	29.50%	3.983%
16	11.380	1579	1580	1583	rVB	58212	29439	1.35%	0.182%
17	11.880	1662	1665	1670	rBV2	165660	148757	6.80%	0.918%
18	11.969	1677	1680	1683	rBV2	20113	22917	1.05%	0.141%
19	12.568	1779	1782	1786	rBV	138449	129419	5.92%	0.799%
20	12.610	1786	1789	1792	rVV2	36564	31943	1.46%	0.197%
21	12.668	1796	1799	1806	rBV5	29665	37444	1.71%	0.231%
22	12.798	1816	1821	1827	rVB2	117513	126616	5.79%	0.782%
23	12.945	1842	1846	1850	rVB	2302504	2067587	94.55%	12.765%
24	13.021	1854	1859	1862	rBV5	16098	26703	1.22%	0.165%
25	13.080	1866	1869	1871	rBV	30024	24915	1.14%	0.154%
26	13.415	1922	1926	1930	rBV5	18481	25870	1.18%	0.160%
27	13.515	1939	1943	1946	rBV6	21542	32635	1.49%	0.201%
28	13.845	1996	1999	2007	rBV	131850	171085	7.82%	1.056%
29	13.998	2020	2025	2028	rBV	609248	656714	30.03%	4.055%
30	14.027	2028	2030	2032	rVB	54882	44550	2.04%	0.275%
31	14.468	2103	2105	2110	rBV5	28889	50210	2.30%	0.310%
32	14.757	2151	2154	2161	rBV2	104692	151630	6.93%	0.936%
33	15.033	2199	2201	2205	rBV	41702	68806	3.15%	0.425%
34	15.398	2261	2263	2266	rVB	36773	33107	1.51%	0.204%
35	15.462	2270	2274	2284	rVB	333429	432881	19.80%	2.673%

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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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

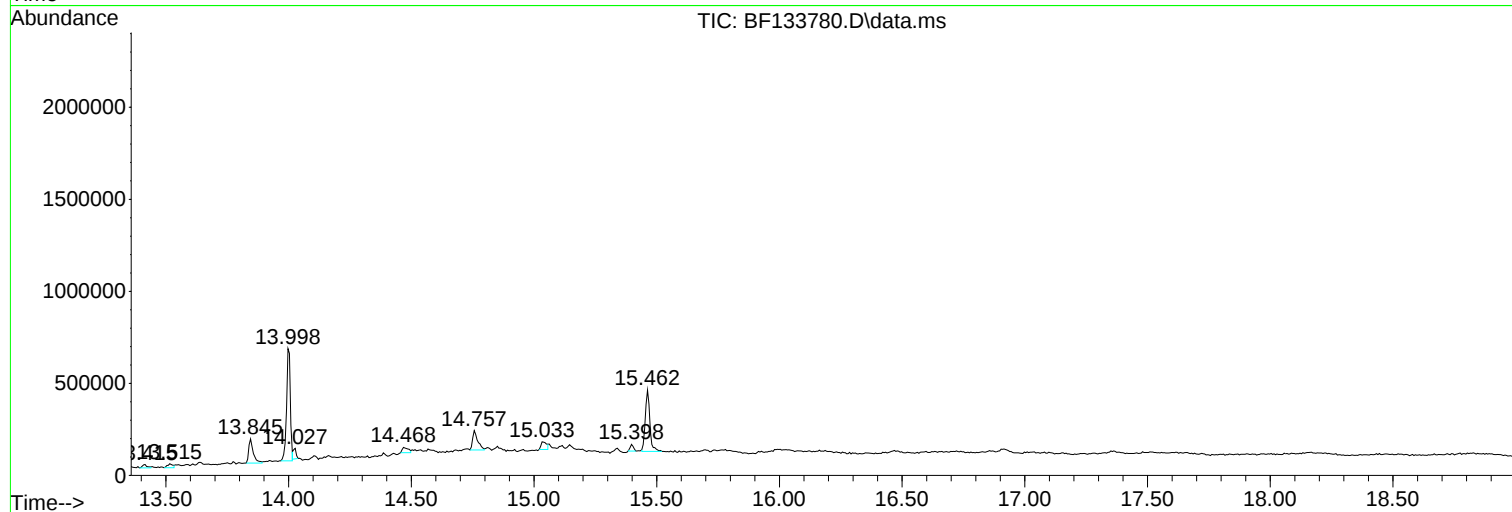
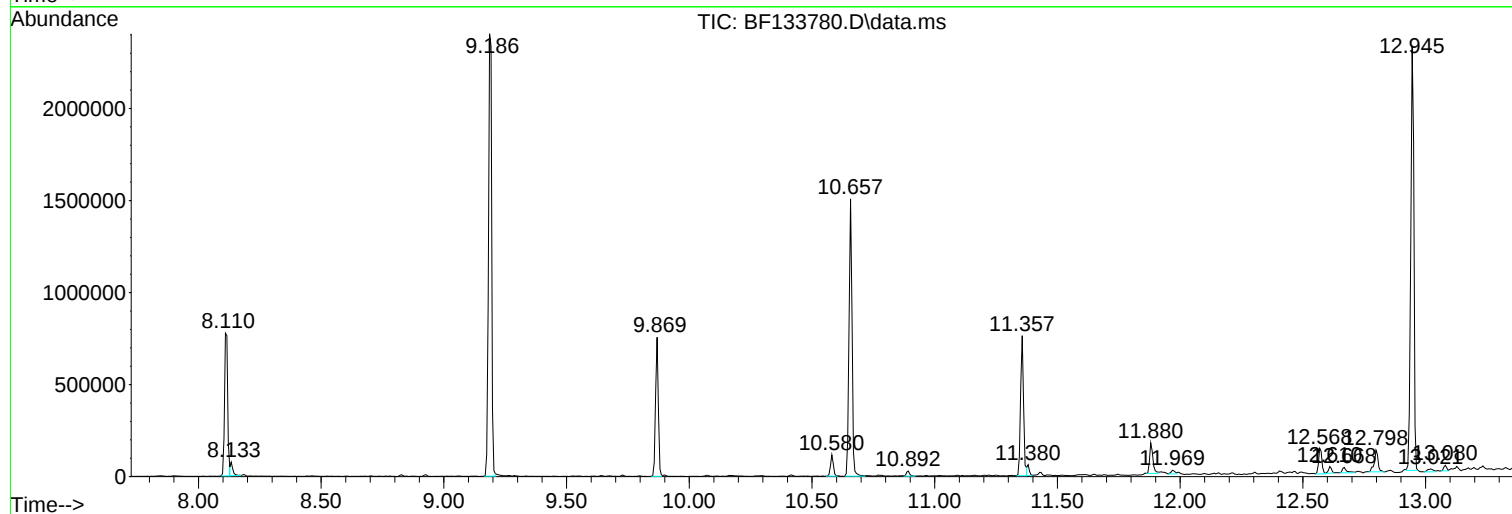
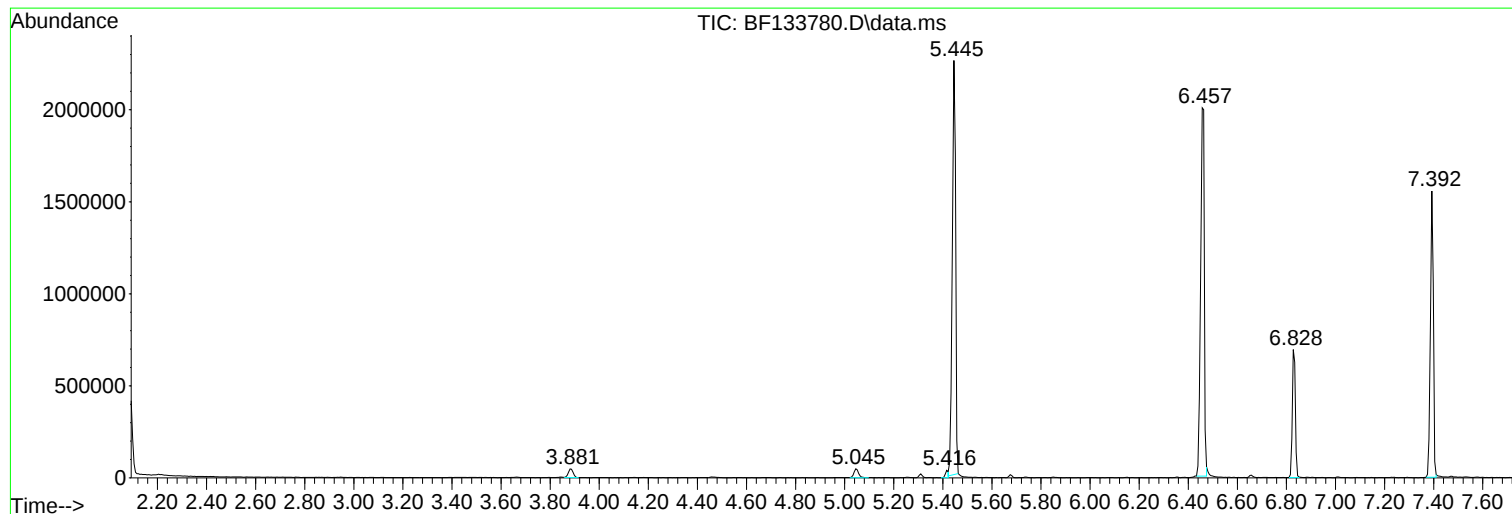
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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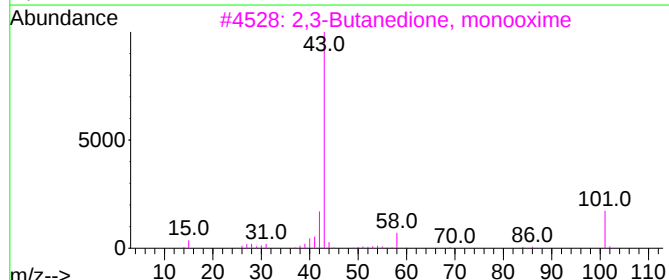
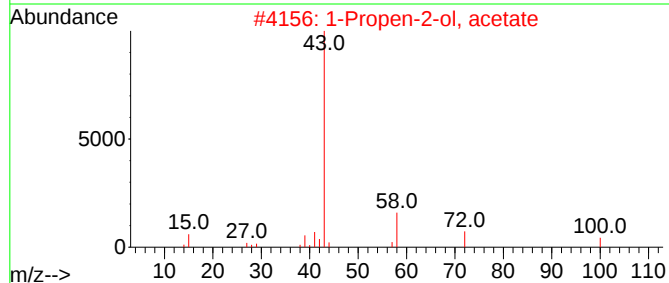
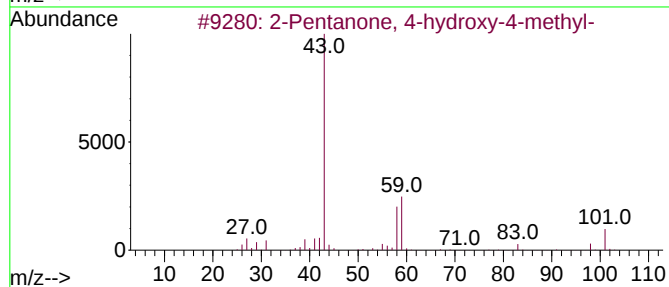
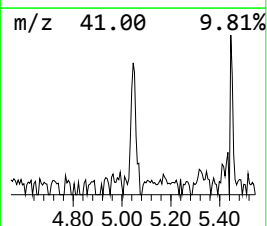
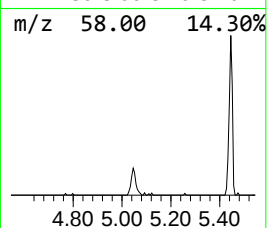
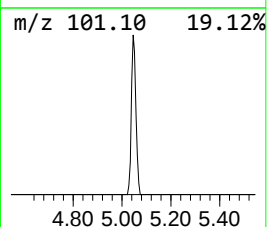
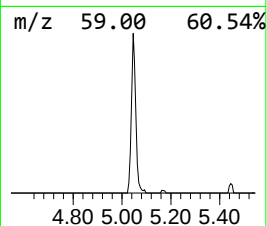
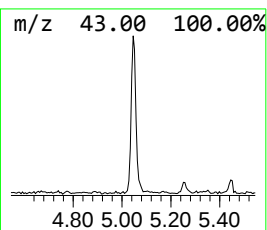
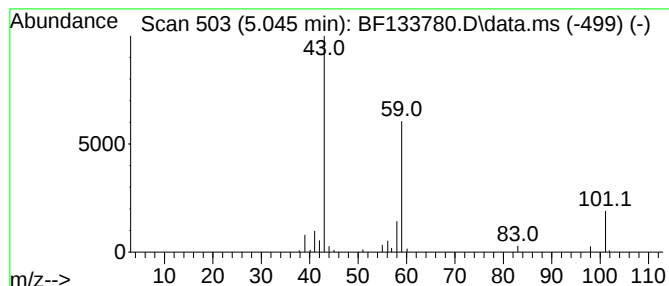
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	2.11 ng	63232	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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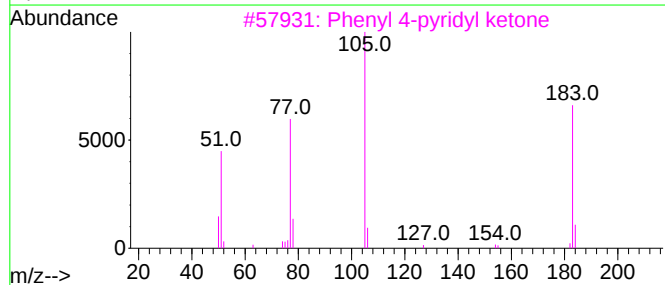
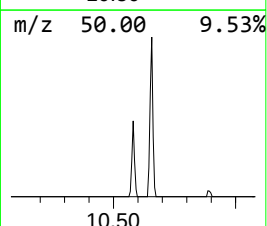
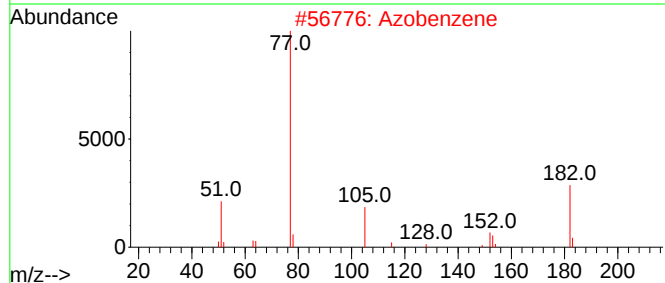
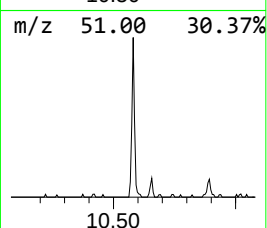
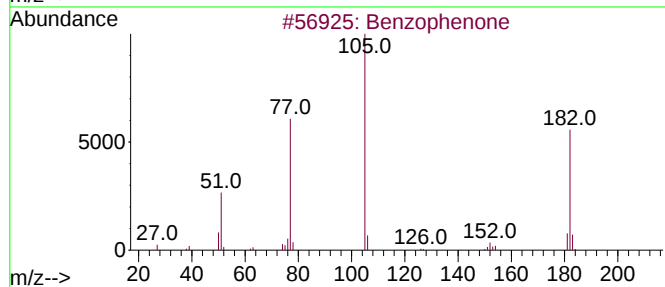
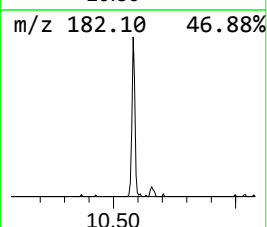
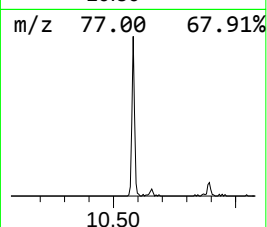
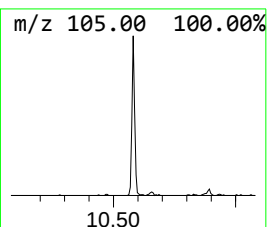
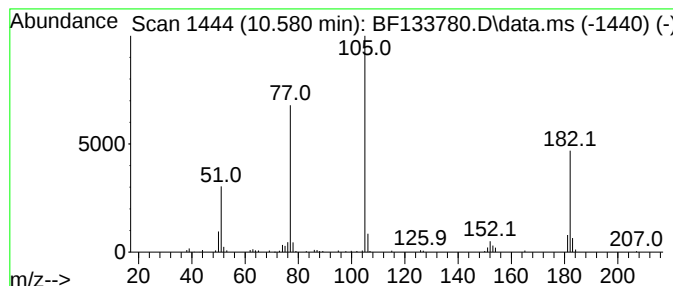
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	3.14 ng	92856	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	58
5			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	49



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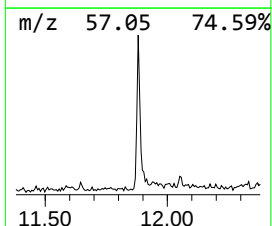
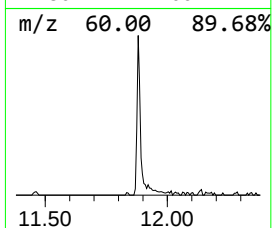
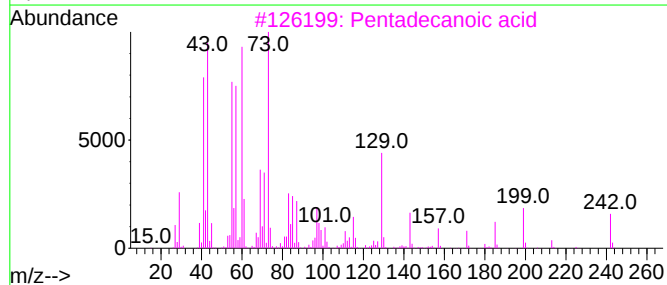
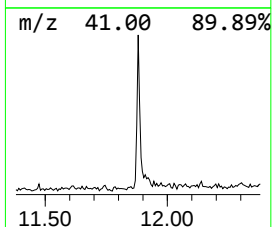
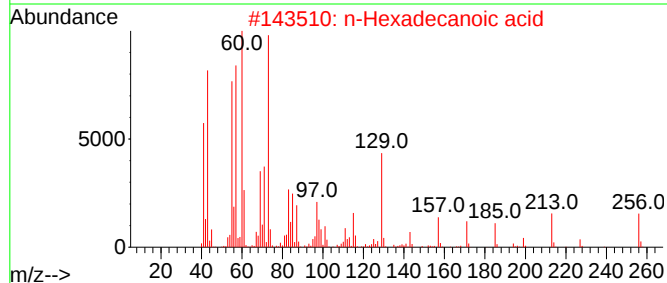
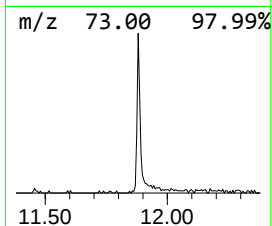
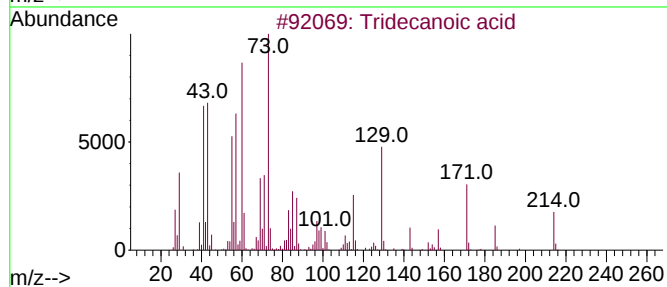
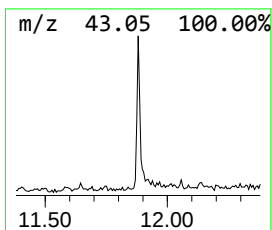
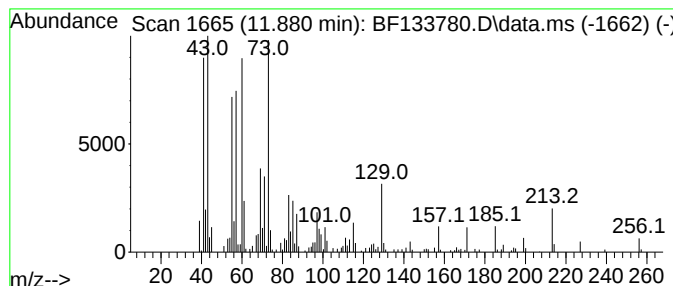
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	4.61 ng	148757	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	94
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Dodecanoic acid	200	C12H24O2	000143-07-7	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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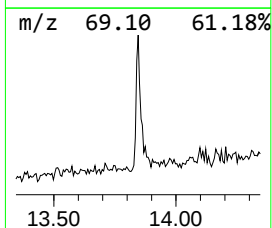
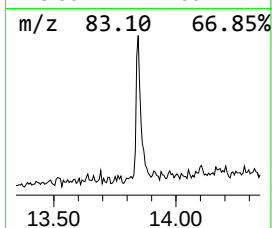
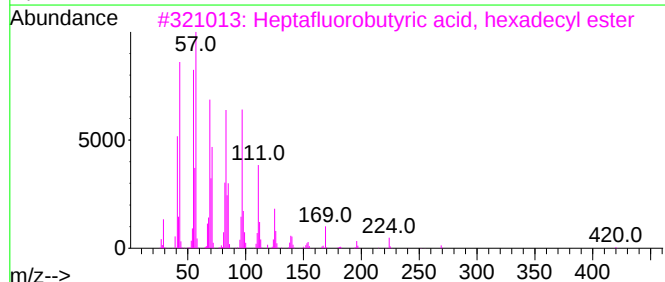
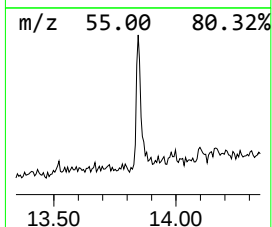
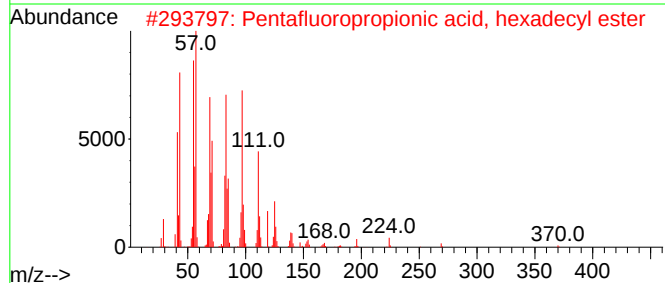
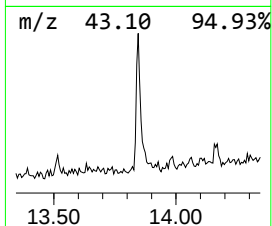
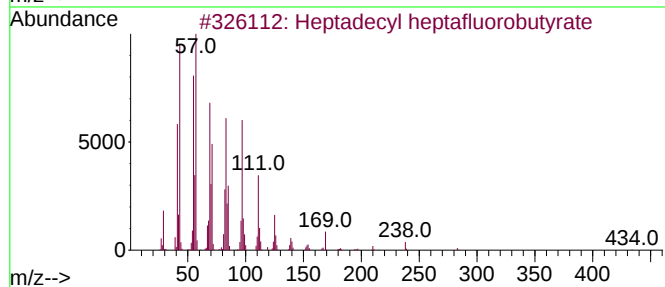
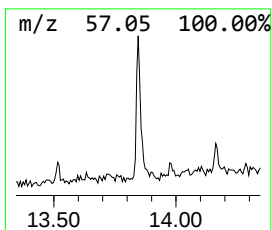
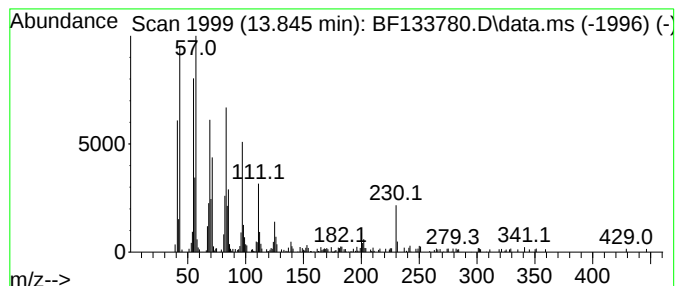
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	5.21 ng	171085	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	87
3			Heptafluorobutyric acid, hexadecyl ester	438	C20H33F7O2	006385-15-5	87
4			Pentafluoropropionic acid, heptadecyl ester	402	C20H35F5O2	959218-78-1	87
5			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87



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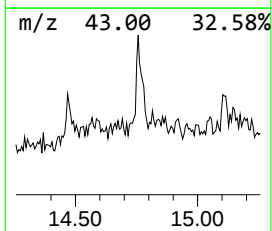
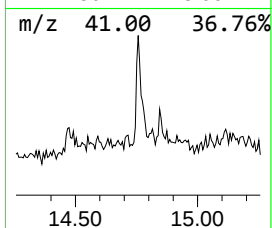
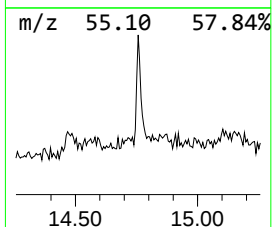
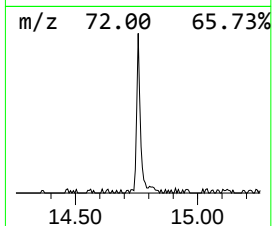
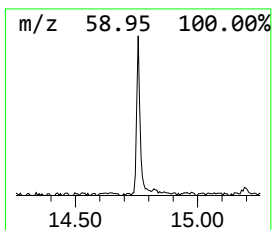
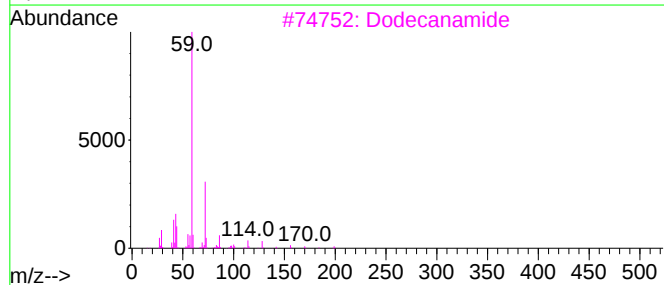
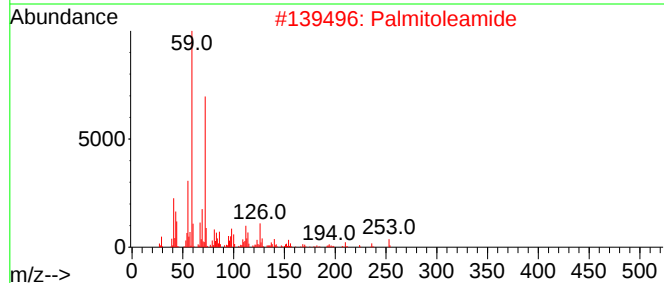
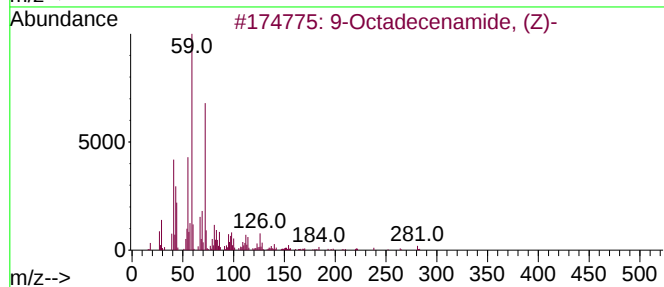
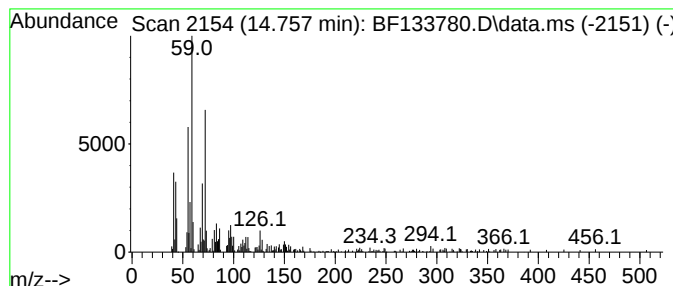
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	7.01 ng	151630	Perylene-d12	15.462

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Palmitoleamide	253	C16H31NO	106010-22-4	78
3		Dodecanamide	199	C12H25NO	001120-16-7	53
4		Bis(dodecanamido)methane	691	C45H90N2O2	010436-15-4	53
5		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
Data File : BF133780.D
Acq On : 15 Jun 2023 17:55
Operator : CG\JU
Sample : 03140-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3-GA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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
2-Pentanone, 4-...	5.045	2.1	ng	63232	1	6.834	600608	20.0
Benzophenone	10.580	3.1	ng	92856	3	9.869	591048	20.0
Tridecanoic acid	11.880	4.6	ng	148757	4	11.357	645165	20.0
Heptadecyl hept...	13.845	5.2	ng	171085	5	14.004	656714	20.0
9-Octadecenamid...	14.757	7.0	ng	151630	6	15.462	432881	20.0