

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072220\
 Data File : BF120973.D
 Acq On : 22 Jul 2020 19:40
 Operator : JU/CG
 Sample : L3361-11
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TW-1

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF071620.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.875	129	134	145	rVB	89091	150600	2.77%	0.461%
2	4.663	435	438	457	rBV2	29879	55938	1.03%	0.171%
3	5.022	496	499	507	rVB	150103	174735	3.21%	0.535%
4	5.428	563	568	571	rBV	2877020	2775850	51.07%	8.492%
5	6.440	728	740	743	rBV	2100359	2069756	38.08%	6.332%
6	6.645	772	775	779	rVB	150308	141848	2.61%	0.434%
7	6.740	788	791	797	rBV	75431	78625	1.45%	0.241%
8	6.810	800	803	807	rBV	1277190	1015007	18.67%	3.105%
9	7.375	893	899	902	rBV	2748751	2821711	51.91%	8.632%
10	7.463	909	914	928	rVB3	46537	82168	1.51%	0.251%
11	7.822	974	975	995	rVB	46634	65120	1.20%	0.199%
12	8.092	1017	1021	1025	rBV	1500849	1332842	24.52%	4.077%
13	8.439	1073	1080	1088	rBV	78731	110452	2.03%	0.338%
14	9.175	1199	1205	1208	rBV	4326007	4779014	87.92%	14.619%
15	9.563	1267	1271	1280	rVB	259383	224529	4.13%	0.687%
16	9.845	1315	1319	1330	rVB	1630616	1608279	29.59%	4.920%
17	10.239	1381	1386	1388	rBV2	160718	214373	3.94%	0.656%
18	10.257	1388	1389	1401	rVB2	125505	123992	2.28%	0.379%
19	10.639	1448	1454	1457	rBV	2833106	3103109	57.09%	9.493%
20	11.333	1567	1572	1575	rBV	1817095	1714542	31.54%	5.245%
21	11.504	1597	1601	1608	rBV2	266690	261456	4.81%	0.800%
22	11.716	1635	1637	1643	rBV2	69610	64537	1.19%	0.197%
23	11.863	1658	1662	1665	rBV	56695	57195	1.05%	0.175%
24	12.922	1837	1842	1845	rBV2	4393096	5435534	100.00%	16.628%
25	13.698	1971	1974	1980	rBV	101205	94115	1.73%	0.288%
26	13.845	1993	1999	2009	rBV2	111786	230808	4.25%	0.706%
27	13.969	2015	2020	2023	rBV	1631000	1622980	29.86%	4.965%
28	14.439	2095	2100	2104	rBV2	57439	60534	1.11%	0.185%
29	14.745	2148	2152	2161	rVB	87726	86317	1.59%	0.264%
30	15.074	2204	2208	2216	rVB	92960	110245	2.03%	0.337%
31	15.415	2260	2266	2270	rBV	1018378	1354621	24.92%	4.144%
32	15.451	2270	2272	2280	rVB	126021	151295	2.78%	0.463%
33	15.874	2339	2344	2351	rBV	95764	134944	2.48%	0.413%
34	16.368	2422	2428	2435	rBV2	76043	135428	2.49%	0.414%

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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

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35	16.945	2520	2526	2534	rBV	50256	99509	1.83%	0.304%
36	17.627	2636	2642	2654	rVB3	34898	88233	1.62%	0.270%
37	18.445	2772	2781	2788	rBV3	20913	59336	1.09%	0.182%

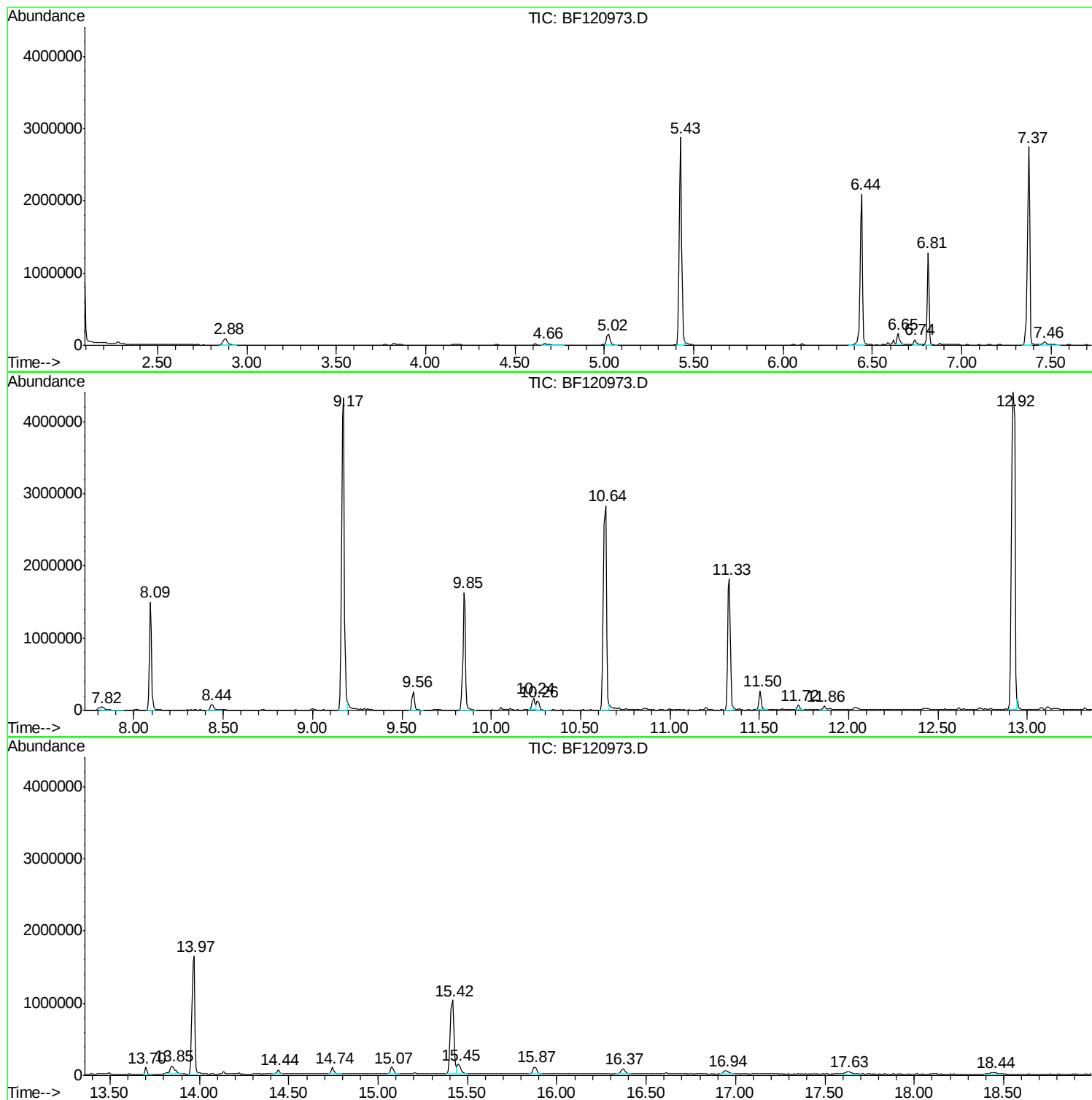
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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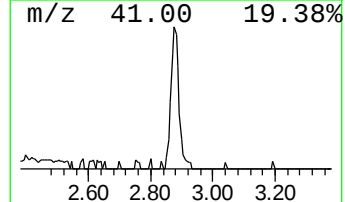
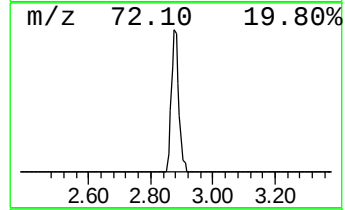
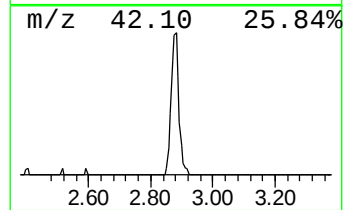
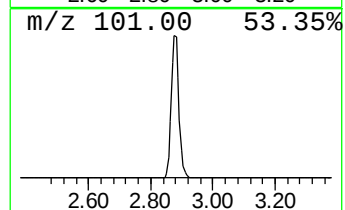
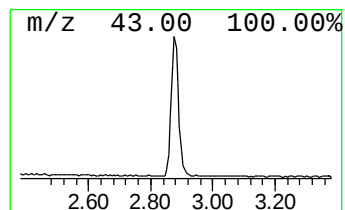
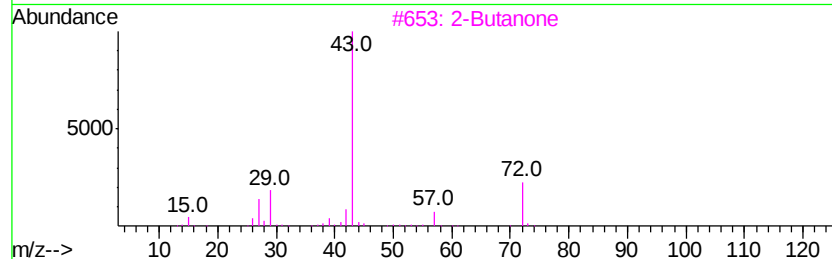
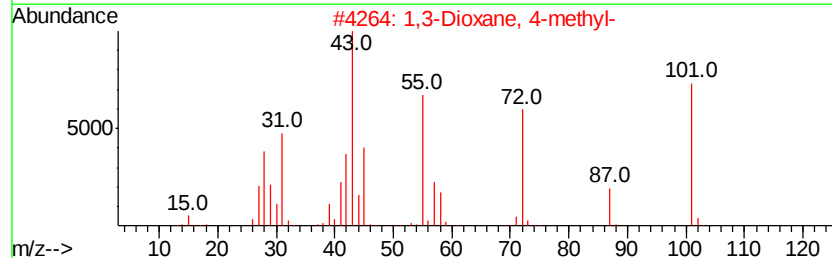
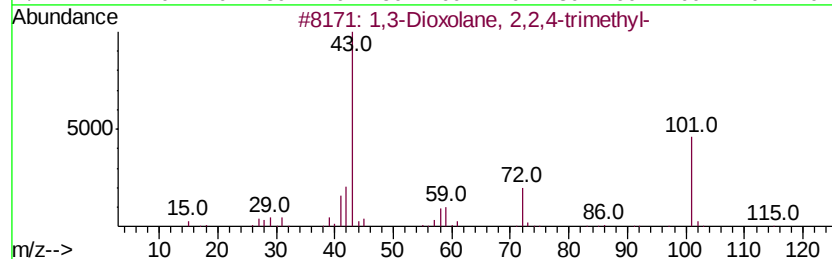
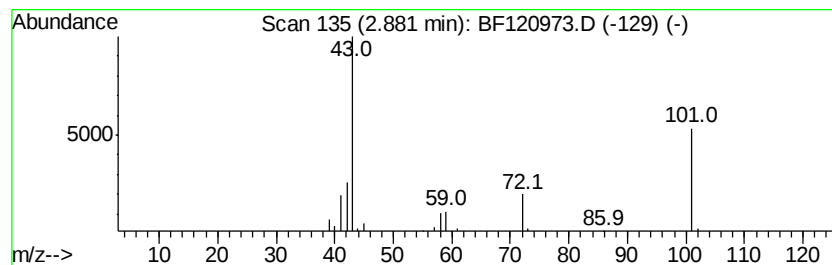
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	2.97 ng	150600	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2			1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	42
3			2-Butanone	72	C4H8O	000078-93-3	9
4			Furazan-3-ol, 4-amino-	101	C2H3N3O2	159013-90-8	9
5			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9



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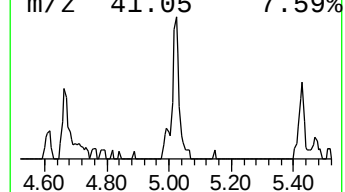
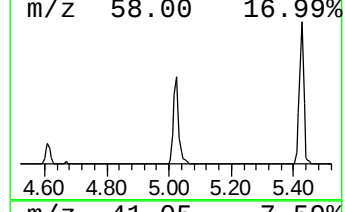
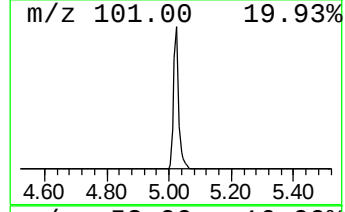
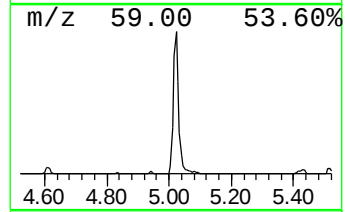
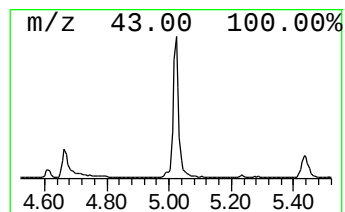
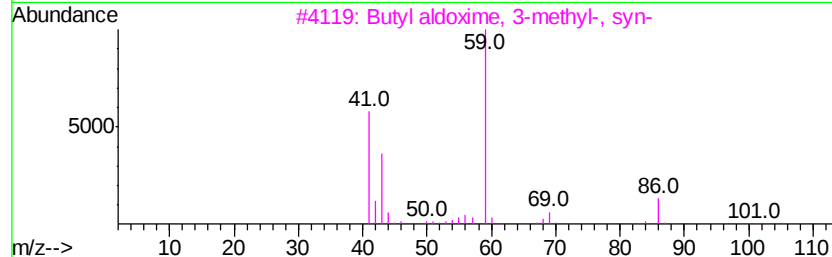
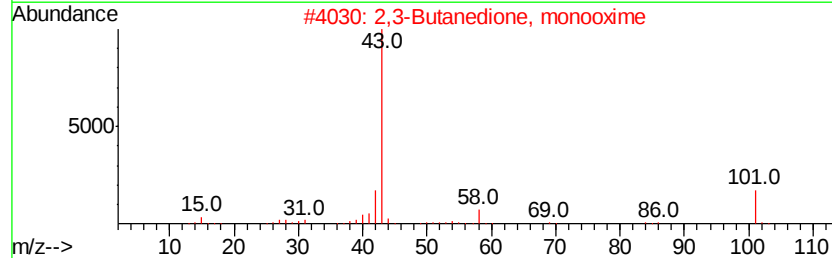
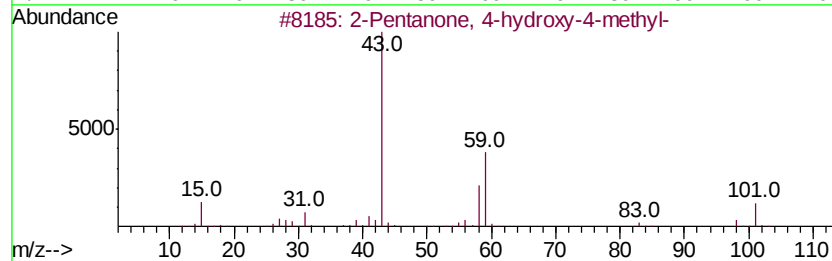
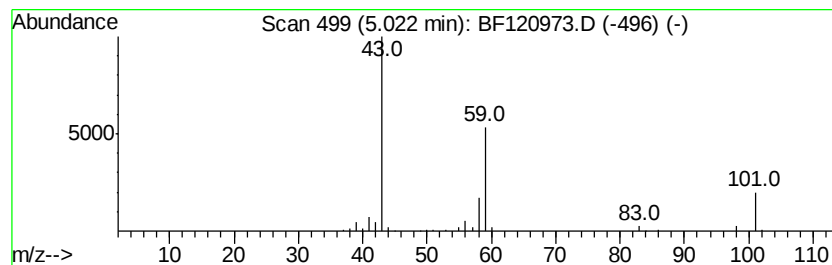
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.44 ng	174735	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
4			Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	9
5			Acetic acid, 1,1-dimethylethyl ester	116	C6H12O2	000540-88-5	9



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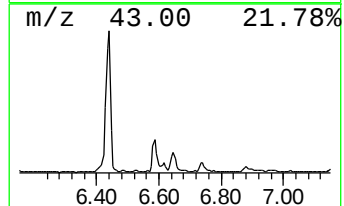
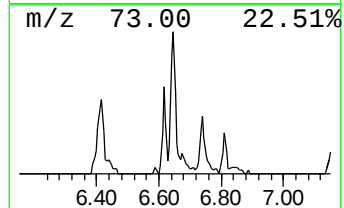
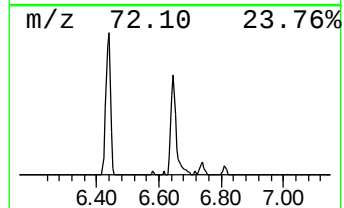
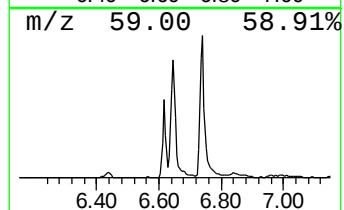
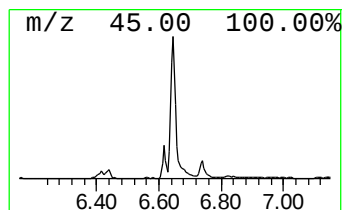
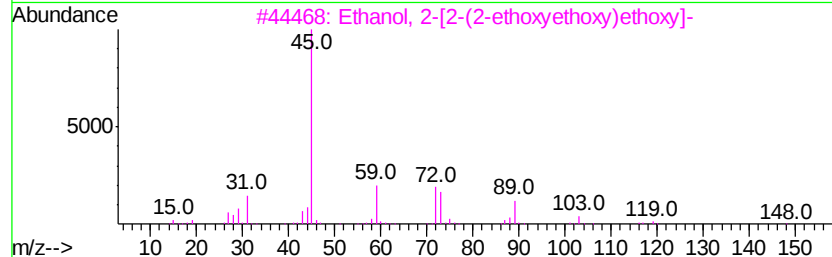
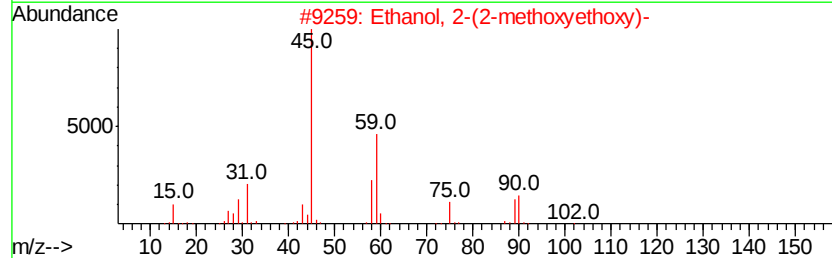
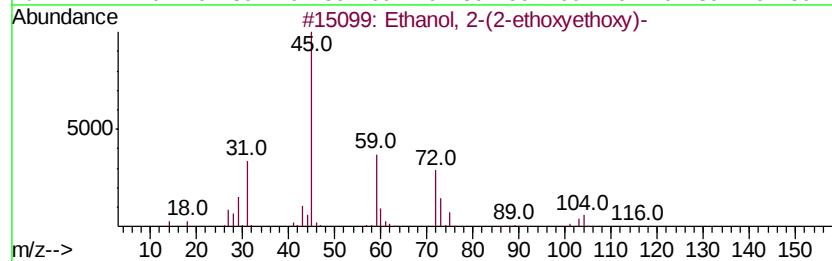
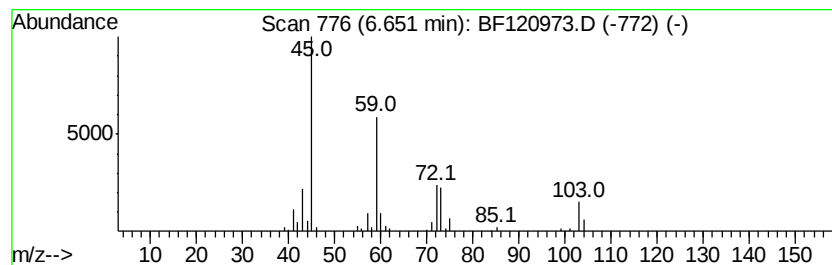
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	2.80 ng	141848	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-ethoxvethoxy)-	134	C6H14O3	000111-90-0	64
2		Ethanol, 2-(2-methoxvethoxy)-	120	C5H12O3	000111-77-3	53
3		Ethanol, 2-[2-(2-ethoxvethoxy)et...	178	C8H18O4	000112-50-5	50
4		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	37
5		2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	32



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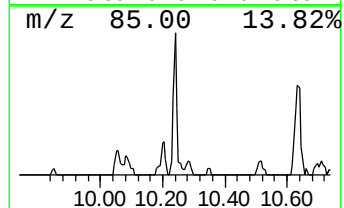
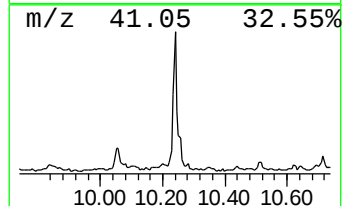
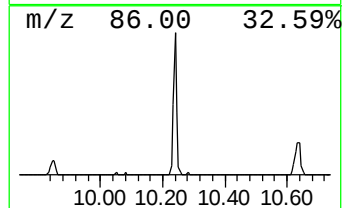
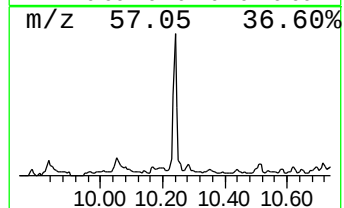
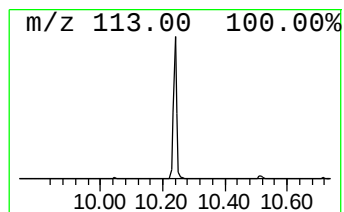
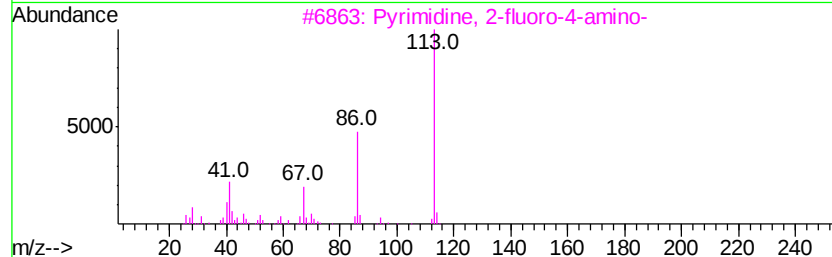
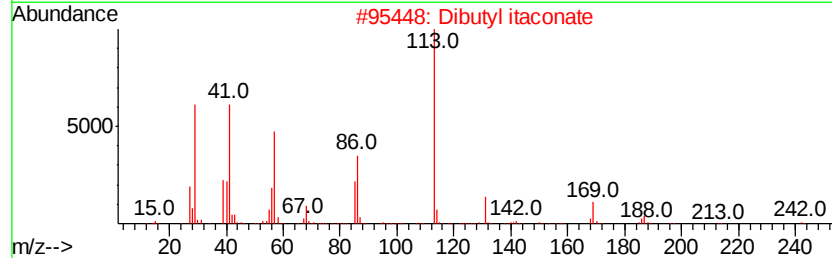
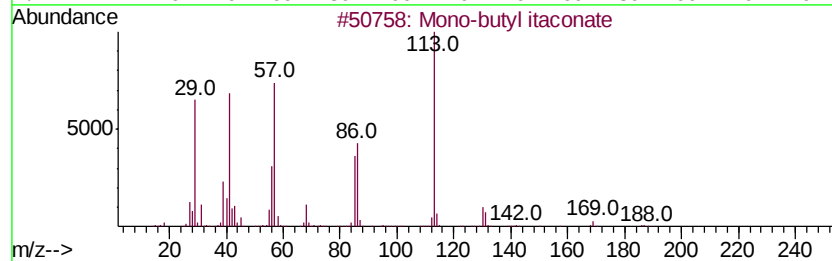
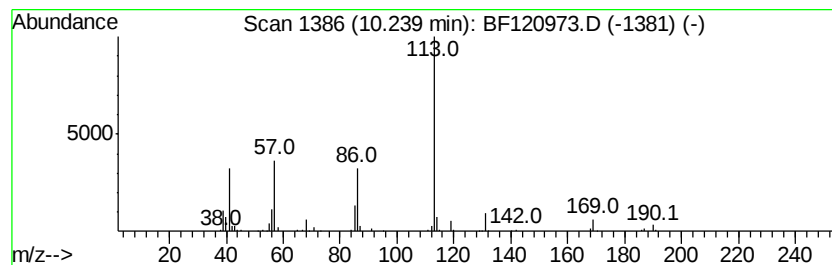
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Mono-butyl itaconate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.24	2.67 ng	214373	Acenaphthene-d10		9.85
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mono-butyl itaconate	186	C9H14O4	006439-57-2	83
2	Dibutyl itaconate	242	C13H22O4	002155-60-4	78
3	Pyrimidine, 2-fluoro-4-amino-	113	C4H4FN3	096548-91-3	58
4	Heptanoic acid, 4-octyl ester	242	C15H30O2	1000160-11-7	45
5	1,5-Diazacyclodecan-2,6-dione	170	C8H14N2O2	1000298-91-2	43



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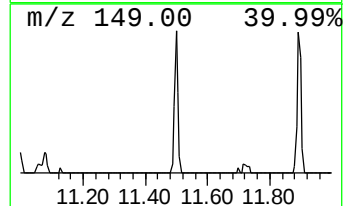
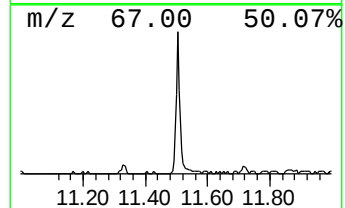
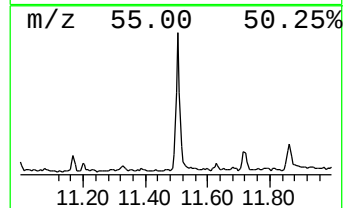
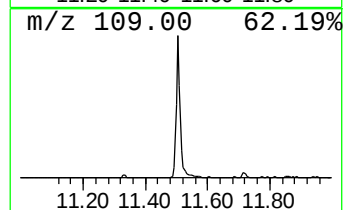
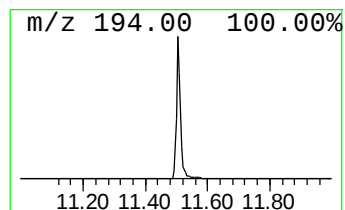
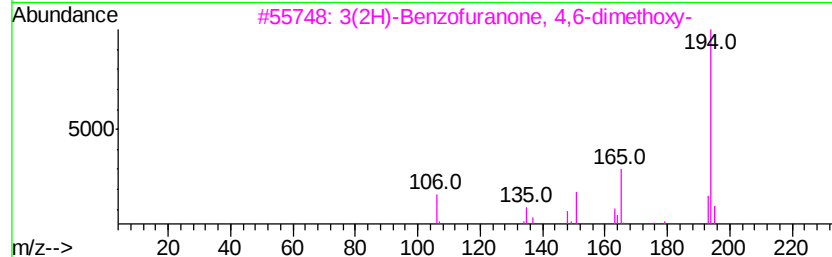
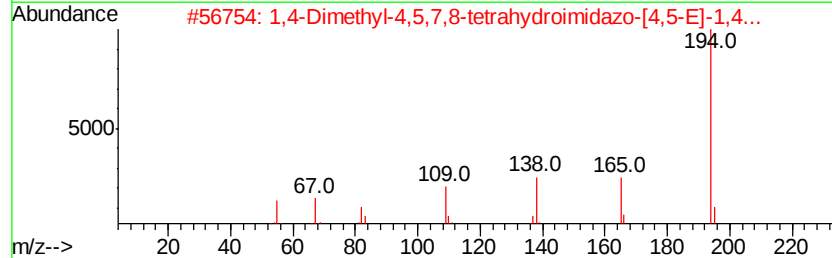
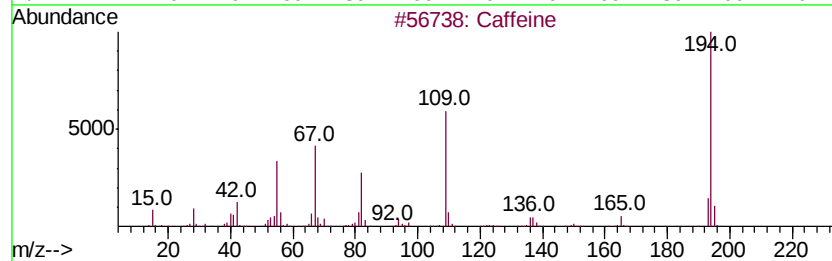
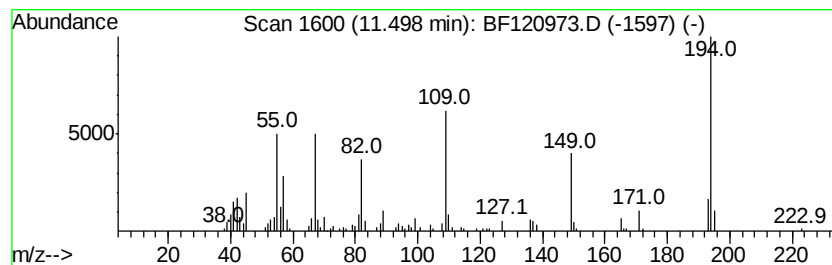
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Caffeine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.50	3.05 ng	261456	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	98
2	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	50
3	3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	50
4	3,3'-Dimethyl-5-methoxy-4,5'-bii...	194	C9H10N2O3	019668-80-5	38
5	7-(Methylthio)pyrimido[4,5-d]pyr...	194	C7H6N4OS	091996-86-0	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072220\
Data File : BF120973.D
Acq On : 22 Jul 2020 19:40
Operator : JU/CG
Sample : L3361-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-1

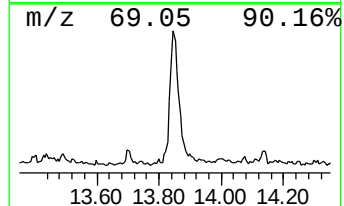
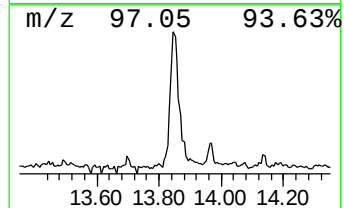
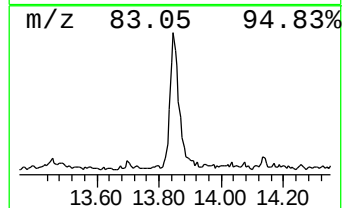
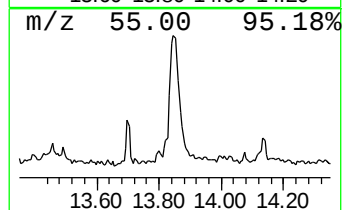
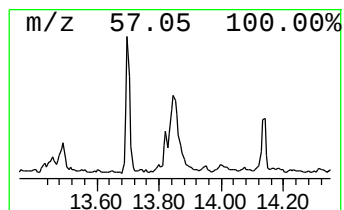
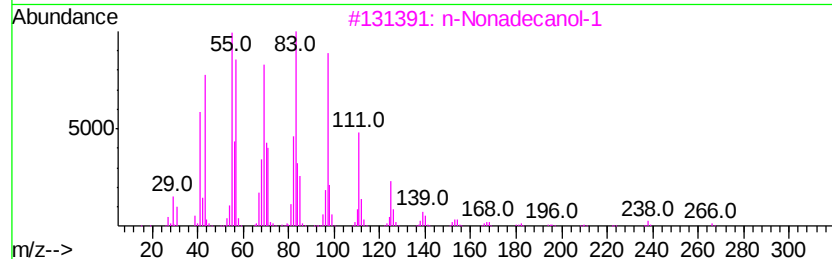
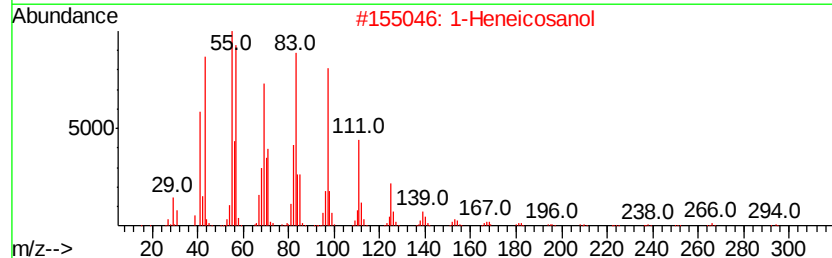
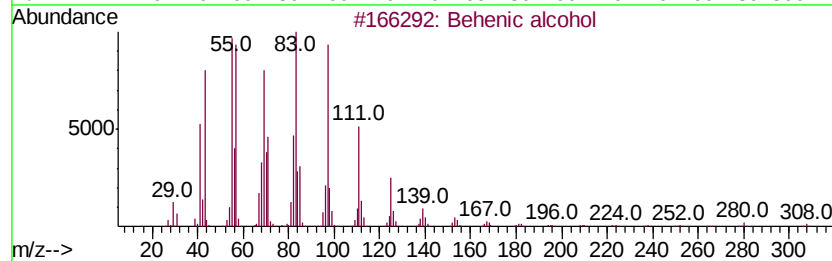
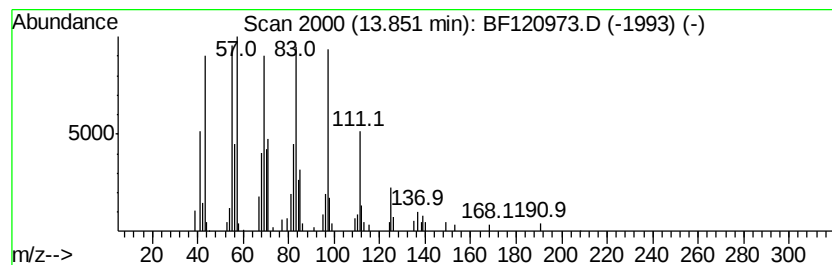
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.84 ng	230808	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072220\
Data File : BF120973.D
Acq On : 22 Jul 2020 19:40
Operator : JU/CG
Sample : L3361-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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
1,3-Dioxolane, 2,...	2.88	3.0	ng	150600	1	6.81	1015010	20.0
2-Pentanone, 4-hy...	5.02	3.4	ng	174735	1	6.81	1015010	20.0
Ethanol, 2-(2-eth...	6.65	2.8	ng	141848	1	6.81	1015010	20.0
Mono-butyl itaconate	10.24	2.7	ng	214373	3	9.85	1608280	20.0
Caffeine	11.50	3.0	ng	261456	4	11.33	1714540	20.0
Behenic alcohol	13.85	2.8	ng	230808	5	13.97	1622980	20.0