

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
 Data File : BF131669.D
 Acq On : 16 Dec 2022 16:32
 Operator : CG\JU
 Sample : N6038-25
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-41-(3-5)

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-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131669.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	15	rVB	342988	441684	22.58%	2.914%
2	5.087	505	510	518	rVB	562118	681185	34.82%	4.494%
3	5.493	575	579	583	rBV	1643140	1527489	78.09%	10.078%
4	6.510	747	752	755	rBV	1717145	1580515	80.80%	10.428%
5	6.881	811	815	818	rBV	490918	413028	21.11%	2.725%
6	7.445	906	911	914	rBV	1165991	1036868	53.01%	6.841%
7	8.169	1030	1034	1037	rBV	653352	517632	26.46%	3.415%
8	9.251	1213	1218	1221	rBV	2154636	1905946	97.44%	12.575%
9	9.933	1330	1334	1337	rBV	669895	595264	30.43%	3.927%
10	10.651	1452	1456	1459	rBV	455032	357310	18.27%	2.357%
11	10.728	1464	1469	1472	rBV	1130032	1061509	54.27%	7.003%
12	11.427	1584	1588	1590	rBV	772736	646683	33.06%	4.267%
13	11.451	1590	1592	1595	rVB	176238	133910	6.85%	0.883%
14	12.251	1726	1728	1731	rVB	32376	23862	1.22%	0.157%
15	12.645	1791	1795	1798	rBV	316289	258160	13.20%	1.703%
16	12.874	1828	1834	1838	rVB	233898	229777	11.75%	1.516%
17	13.022	1854	1859	1862	rVB	2358058	1956111	100.00%	12.906%
18	13.921	2008	2012	2032	rBV4	76962	209799	10.73%	1.384%
19	14.080	2032	2039	2041	rVV	503362	536756	27.44%	3.541%
20	14.104	2041	2043	2048	rVV	84124	72700	3.72%	0.480%
21	14.174	2051	2055	2061	rVB2	33248	44032	2.25%	0.291%
22	14.233	2061	2065	2068	rBV3	27872	30064	1.54%	0.198%
23	14.545	2114	2118	2122	rBV2	31840	34251	1.75%	0.226%
24	14.939	2180	2185	2194	rBV	88195	98218	5.02%	0.648%
25	15.133	2214	2218	2222	rBV	56959	89428	4.57%	0.590%
26	15.210	2227	2231	2235	rVB	34517	36786	1.88%	0.243%
27	15.451	2268	2272	2279	rVB	37257	43751	2.24%	0.289%
28	15.515	2279	2283	2288	rBV	42048	50412	2.58%	0.333%
29	15.580	2289	2294	2303	rBV	306422	392956	20.09%	2.593%
30	16.057	2370	2375	2381	rVB2	18082	30723	1.57%	0.203%
31	16.892	2511	2517	2528	rBV8	13193	33131	1.69%	0.219%
32	17.092	2546	2551	2559	rBV3	22689	46150	2.36%	0.304%
33	17.556	2623	2630	2638	rVB2	19911	40840	2.09%	0.269%

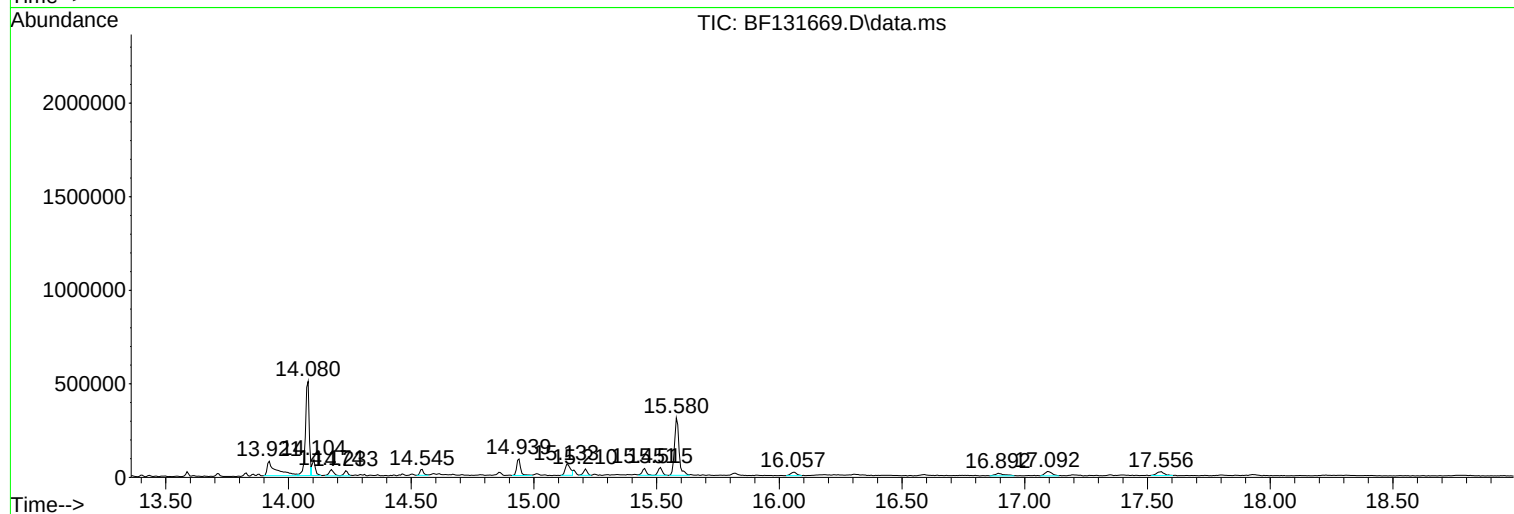
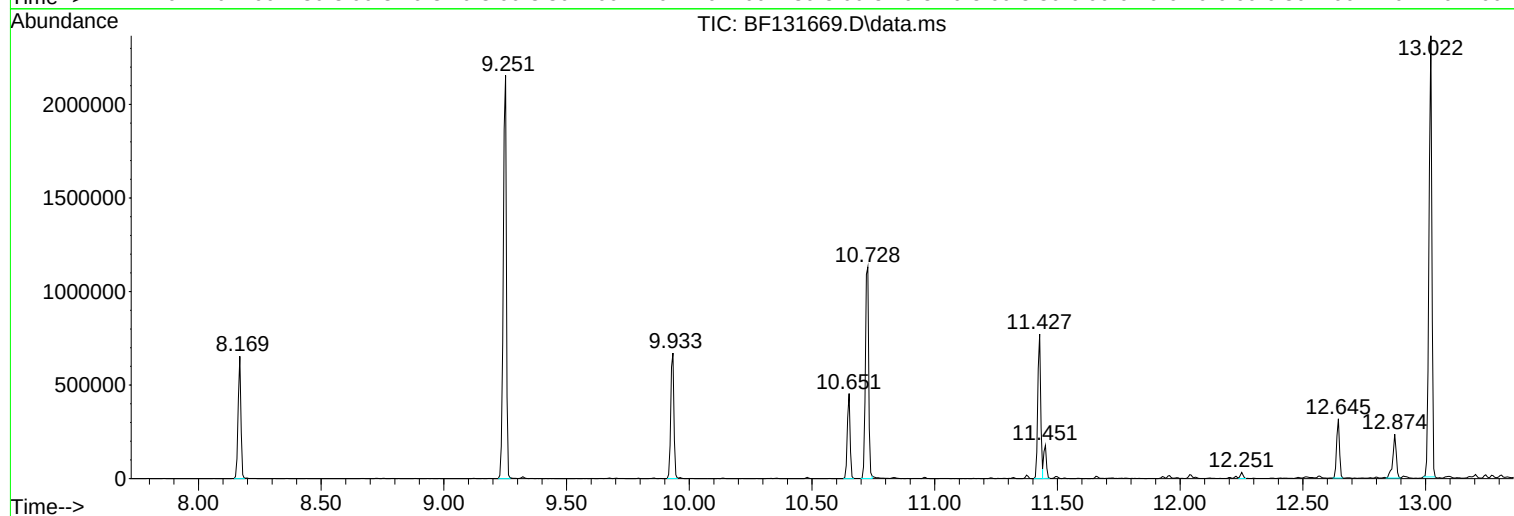
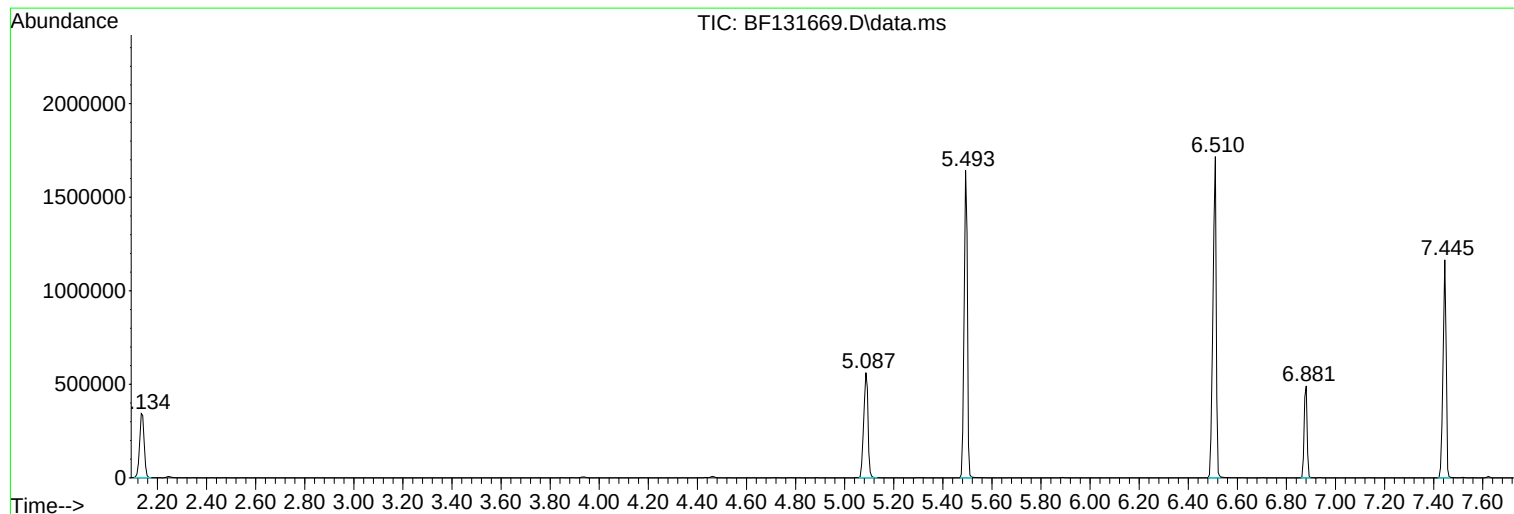
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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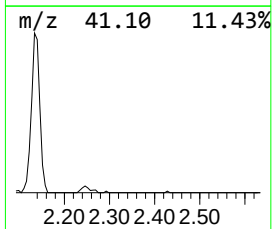
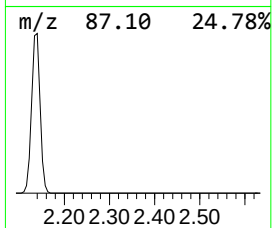
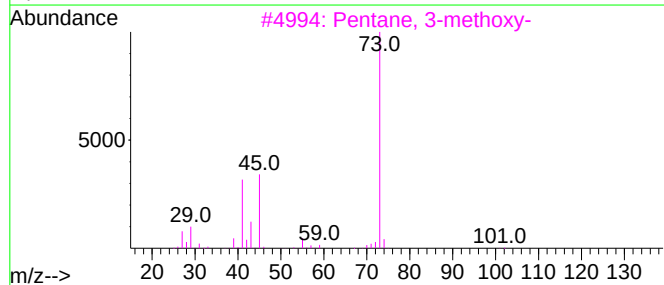
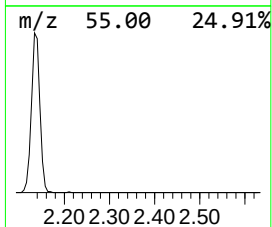
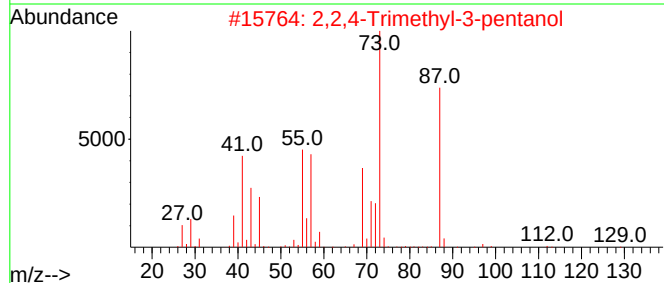
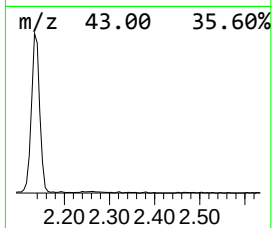
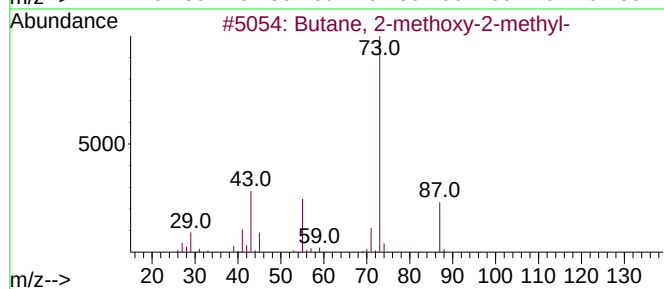
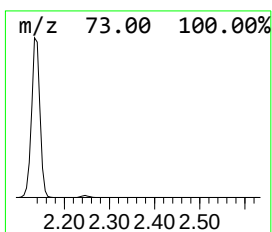
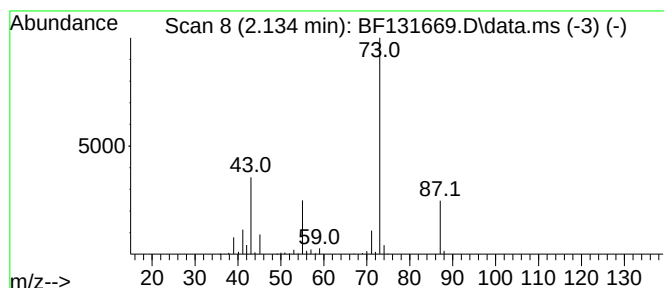
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	21.39 ng	441684	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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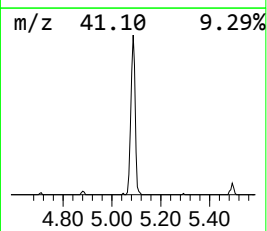
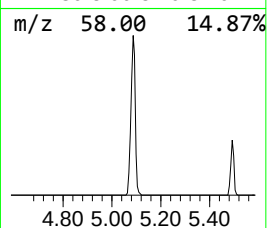
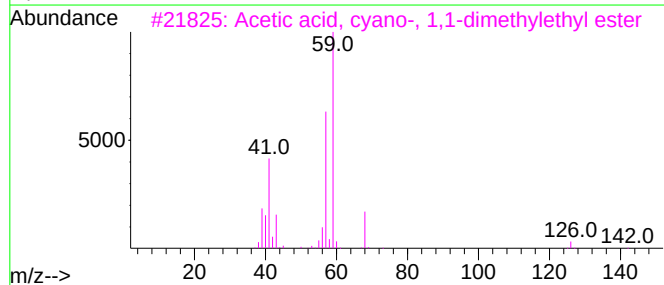
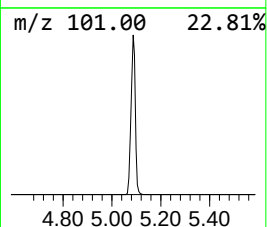
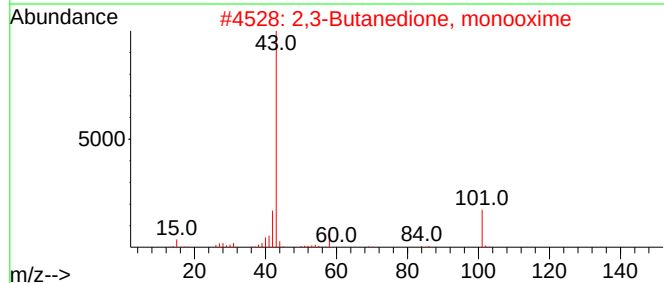
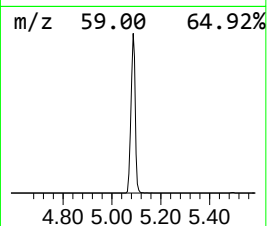
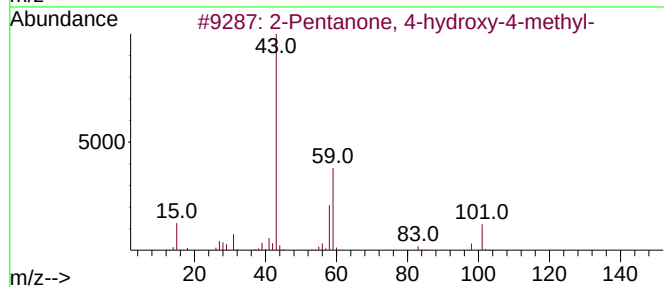
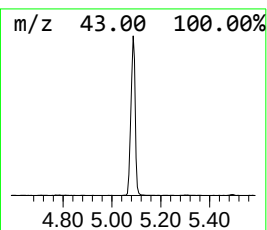
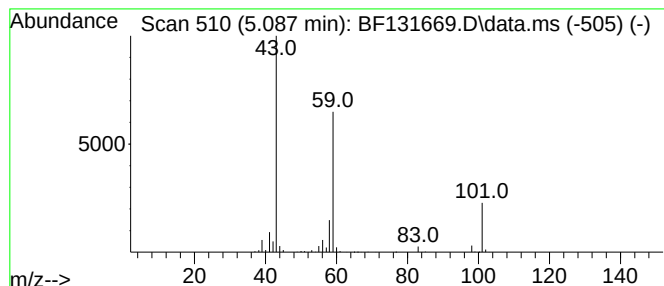
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	32.98 ng	681185	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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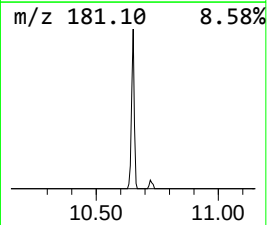
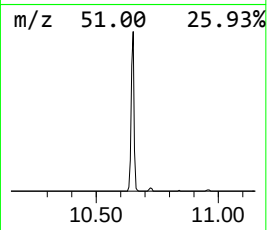
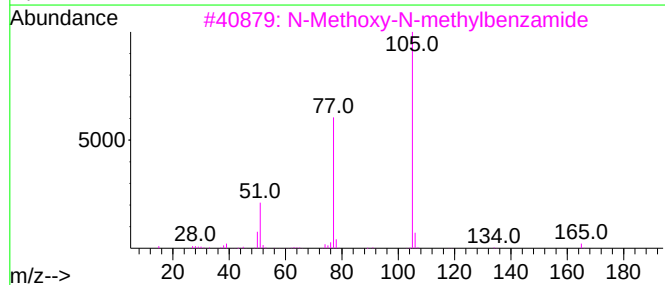
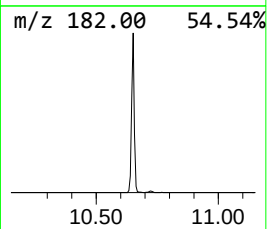
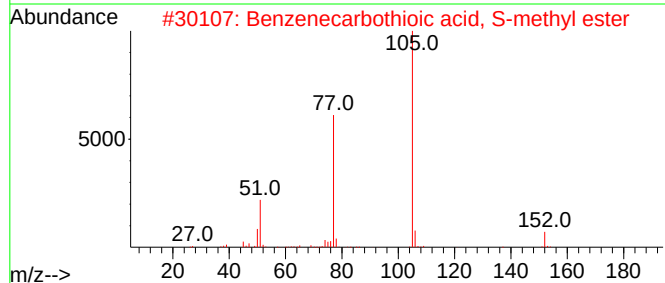
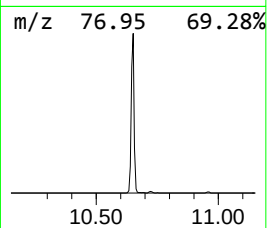
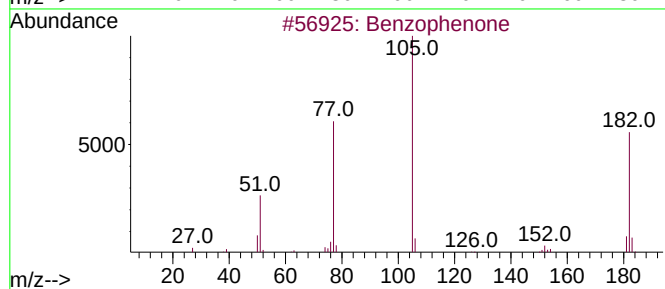
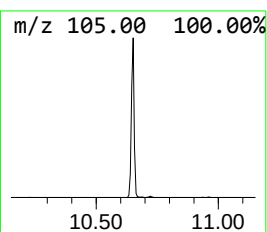
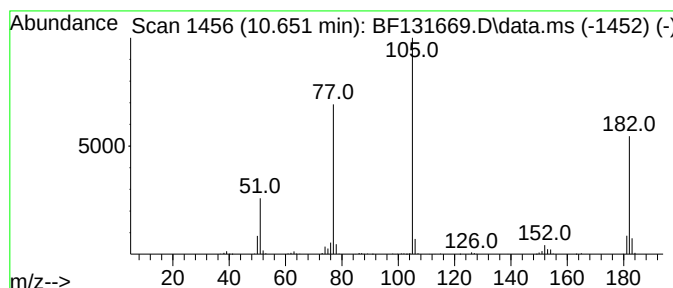
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	12.01 ng	357310	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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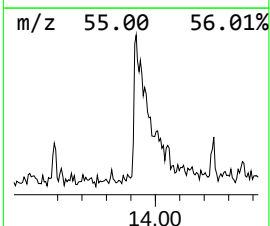
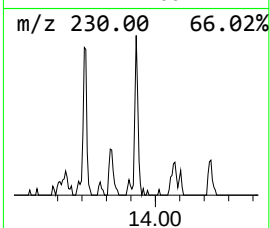
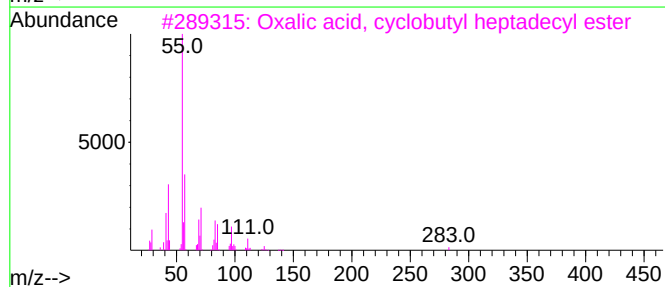
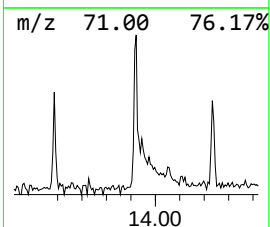
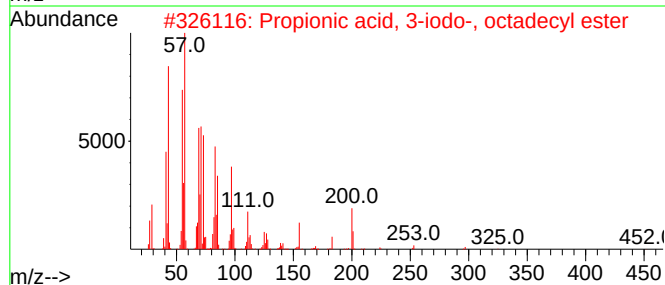
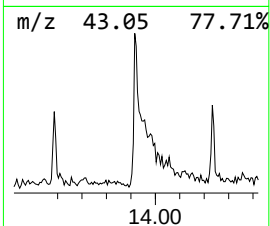
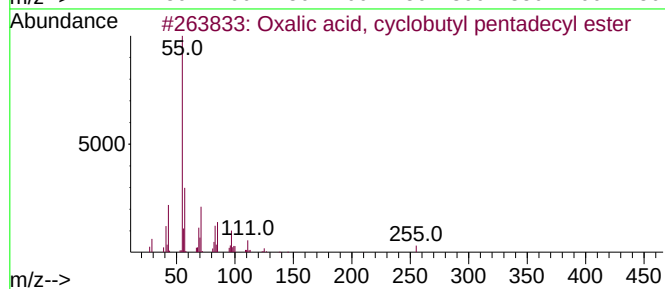
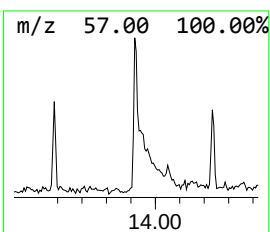
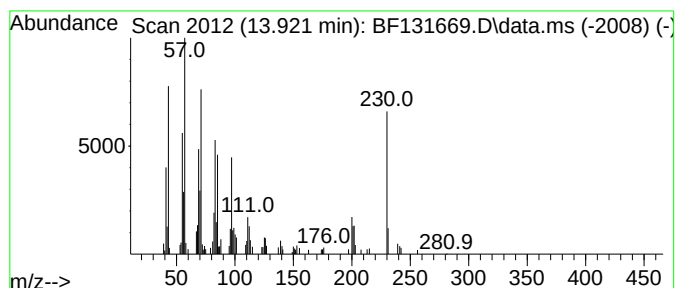
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Peak Number 4 Oxalic acid, cyclobutyl pen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	7.82 ng	209799	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1010309-70-5	70
2			Propionic acid, 3-iodo-, octadec...	452	C21H41IO2	1000406-24-9	68
3			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	64
4			Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	62
5			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	53



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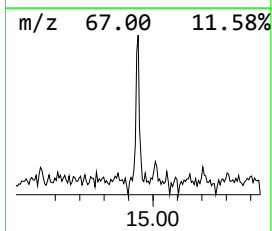
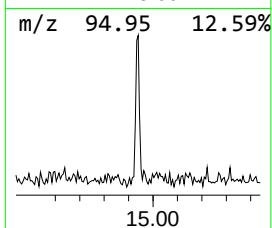
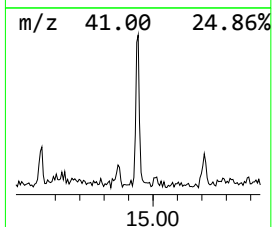
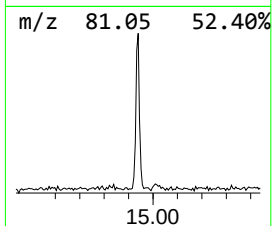
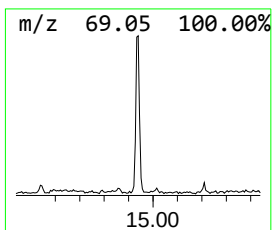
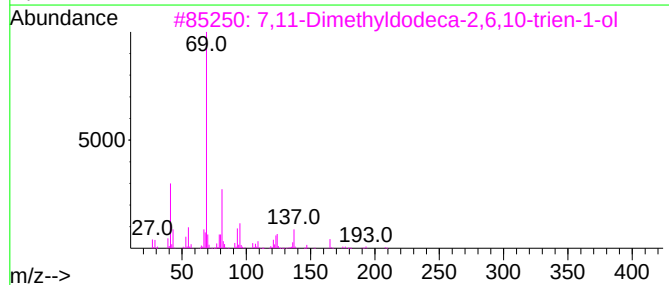
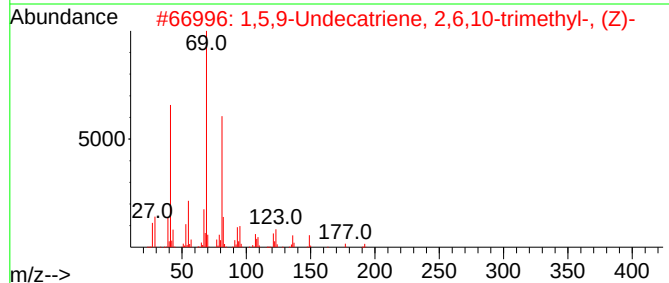
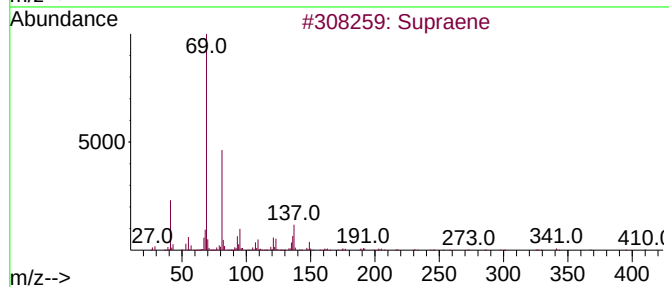
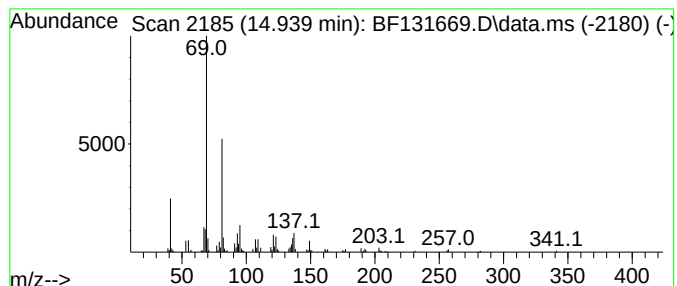
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	5.00 ng	98218	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	86
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64



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ClientSampleId :
RB-41-(3-5)

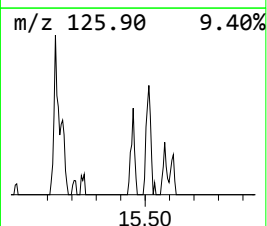
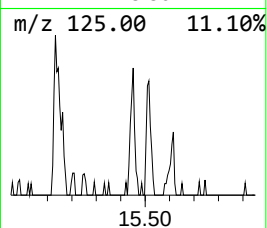
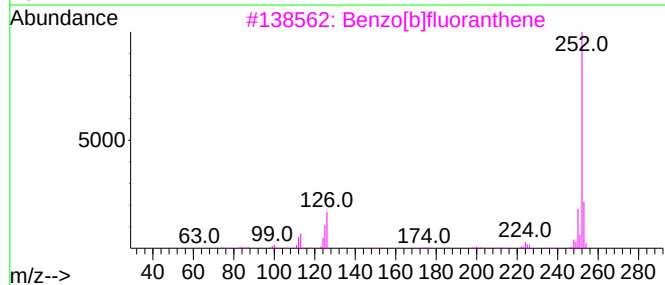
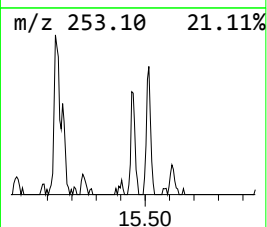
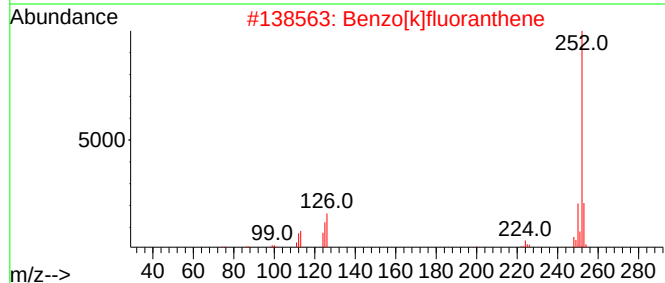
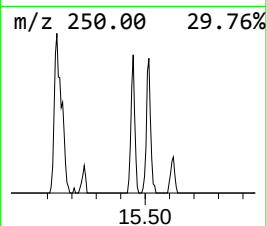
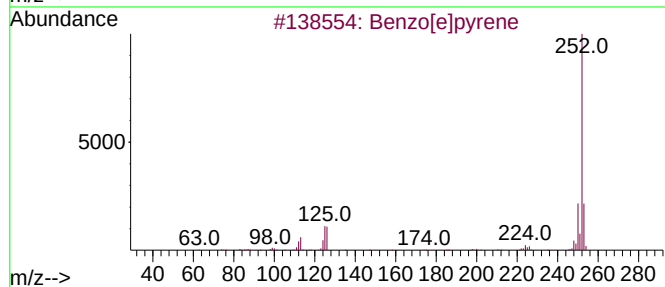
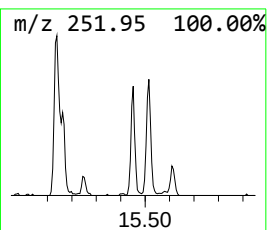
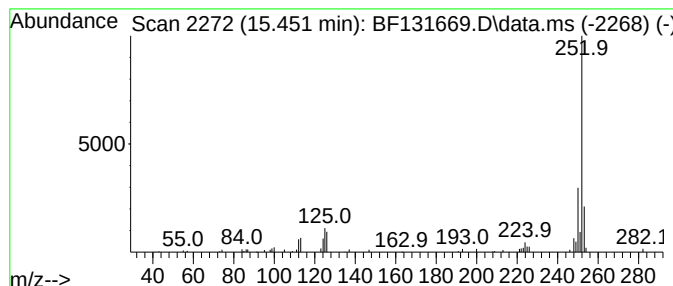
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.451	2.23 ng	43751	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	90
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
Data File : BF131669.D
Acq On : 16 Dec 2022 16:32
Operator : CG\JU
Sample : N6038-25
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-41-(3-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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
Butane, 2-metho...	2.134	21.4	ng	441684	1	6.881	413028	20.0
2-Pentanone, 4-...	5.087	33.0	ng	681185	1	6.881	413028	20.0
Benzophenone	10.651	12.0	ng	357310	3	9.933	595264	20.0
Oxalic acid, cy...	13.921	7.8	ng	209799	5	14.080	536756	20.0
Supraene	14.939	5.0	ng	98218	6	15.580	392956	20.0
Benzo[e]pyrene	15.451	2.2	ng	43751	6	15.580	392956	20.0