

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061923\
 Data File : BF133836.D
 Acq On : 19 Jun 2023 16:31
 Operator : CG\JU
 Sample : 03282-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-NEX-001

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: BF133836.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	7	12	20	rVB	558542	735713	37.03%	4.512%
2	2.275	27	32	37	rVB	32100	41906	2.11%	0.257%
3	3.975	316	321	325	rBV	32112	40086	2.02%	0.246%
4	5.099	507	512	522	rVB	186563	237200	11.94%	1.455%
5	5.493	574	579	582	rBV	2140828	1929952	97.14%	11.837%
6	6.493	744	749	752	rBV	1983232	1986680	100.00%	12.185%
7	6.857	807	811	814	rBV	762211	594793	29.94%	3.648%
8	7.416	902	906	909	rBV	1455885	1306810	65.78%	8.015%
9	8.134	1025	1028	1032	rBV	926643	760974	38.30%	4.667%
10	9.210	1208	1211	1215	rBV	2317830	1929570	97.13%	11.835%
11	9.892	1323	1327	1331	rBV	1015269	796982	40.12%	4.888%
12	10.610	1443	1449	1452	rBV	148437	118048	5.94%	0.724%
13	10.681	1457	1461	1465	rBV	1285430	1236214	62.23%	7.582%
14	11.386	1577	1581	1584	rBV	868447	739094	37.20%	4.533%
15	11.916	1668	1671	1676	rBV	217443	210705	10.61%	1.292%
16	12.604	1783	1788	1791	rBV	30508	36123	1.82%	0.222%
17	12.704	1802	1805	1813	rBV	50998	65138	3.28%	0.400%
18	12.980	1848	1852	1856	rBV	1628291	1364269	68.67%	8.367%
19	13.216	1887	1892	1896	rBV2	22019	30130	1.52%	0.185%
20	13.892	2003	2007	2011	rBV	154090	240447	12.10%	1.475%
21	13.963	2013	2019	2027	rVV9	106394	357730	18.01%	2.194%
22	14.045	2028	2033	2036	rVB	638766	627104	31.57%	3.846%
23	14.210	2059	2061	2064	rVB	31669	25109	1.26%	0.154%
24	14.516	2110	2113	2116	rBV	45358	53657	2.70%	0.329%
25	15.186	2224	2227	2233	rBV2	39463	43265	2.18%	0.265%
26	15.551	2283	2289	2293	rBV	584426	748249	37.66%	4.589%
27	16.051	2372	2374	2382	rVB2	32415	48495	2.44%	0.297%

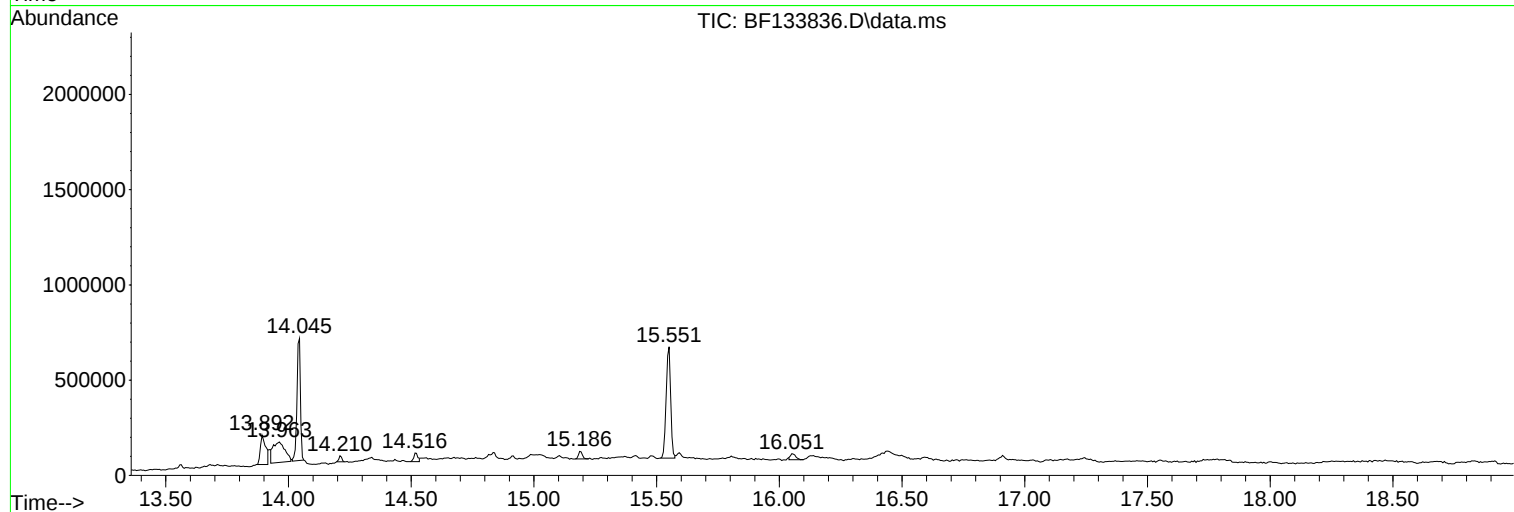
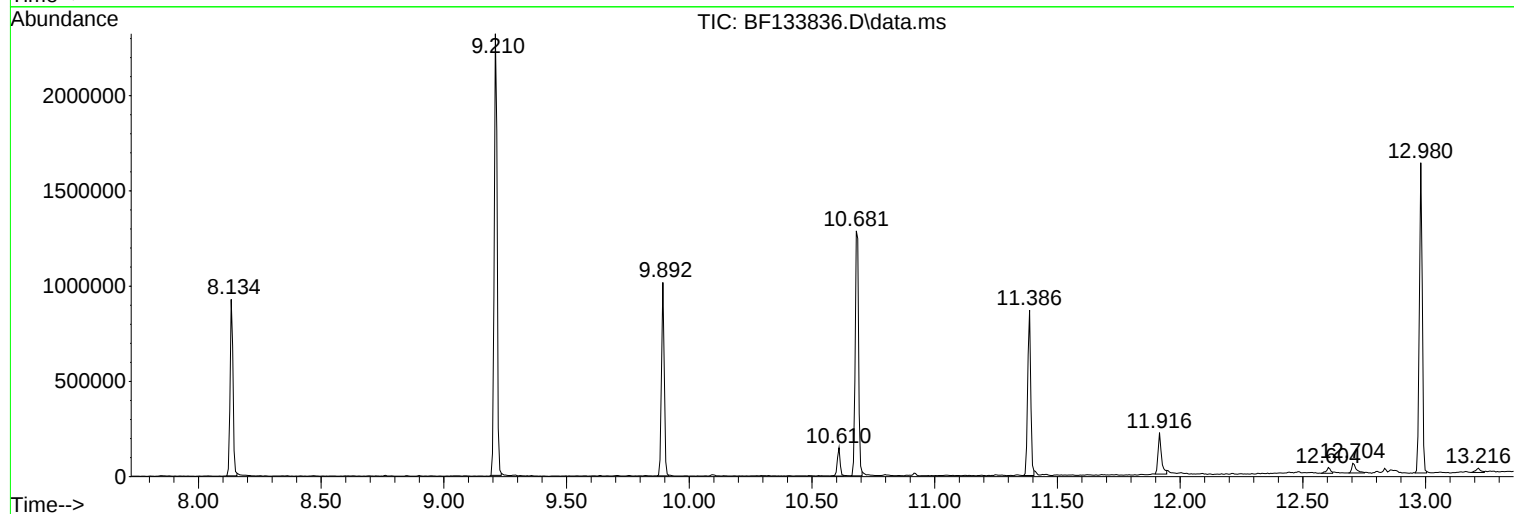
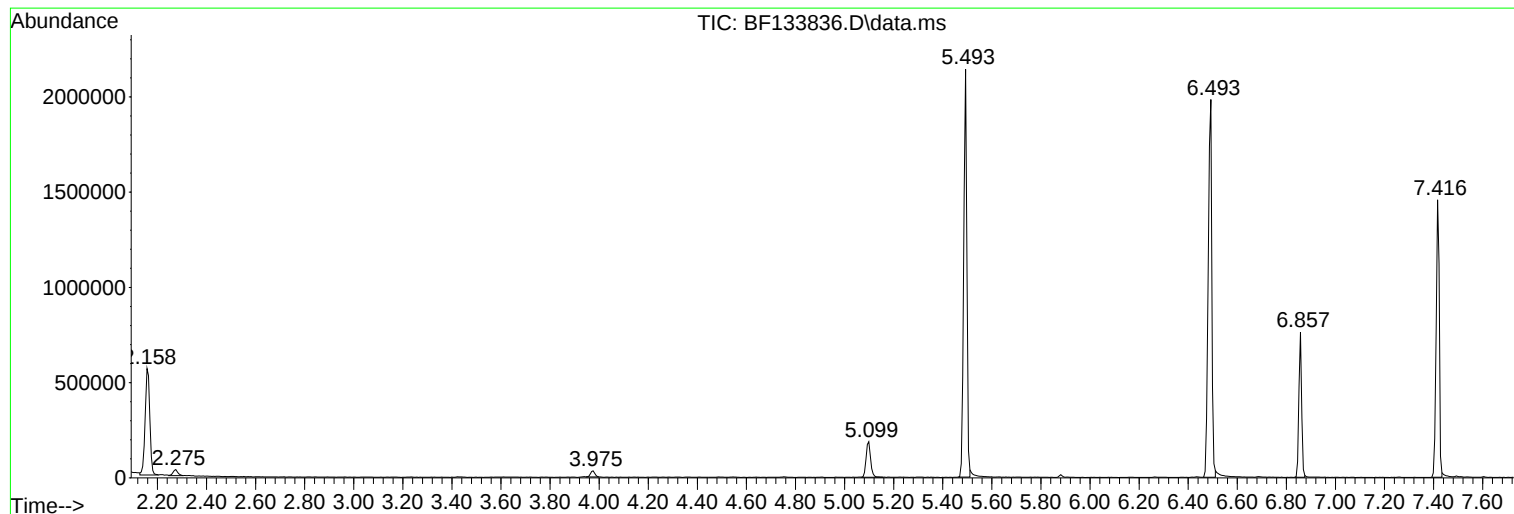
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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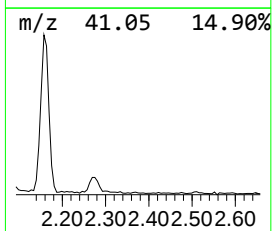
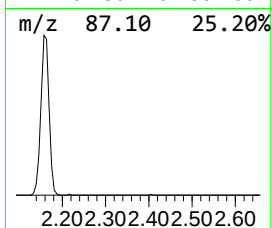
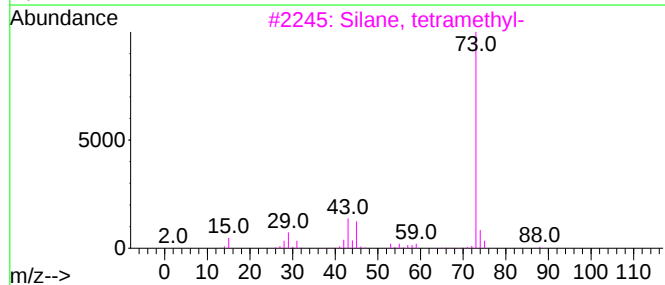
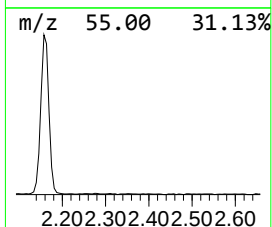
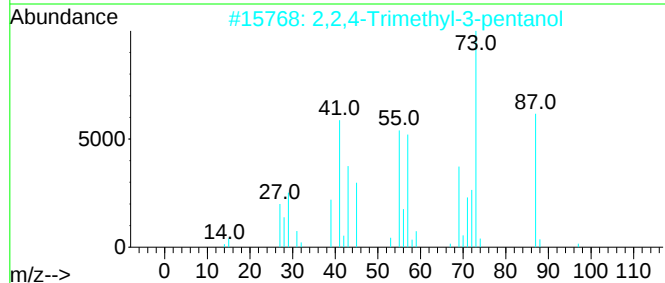
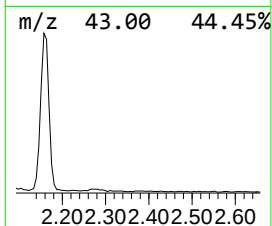
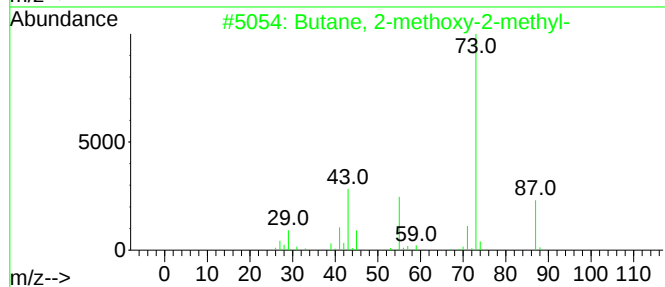
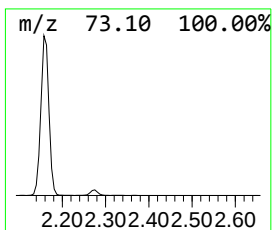
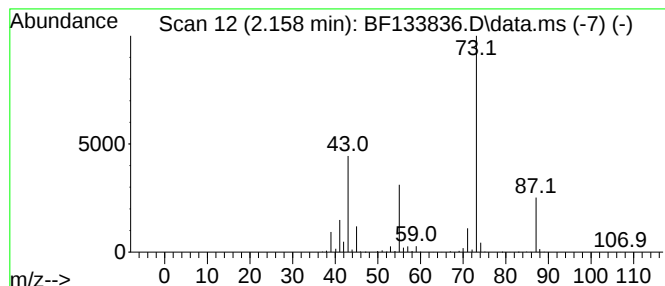
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.158	24.74 ng	735713	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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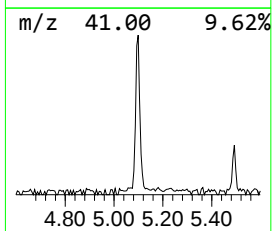
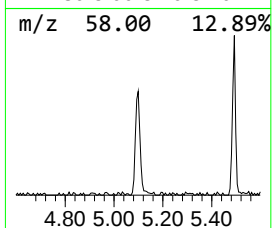
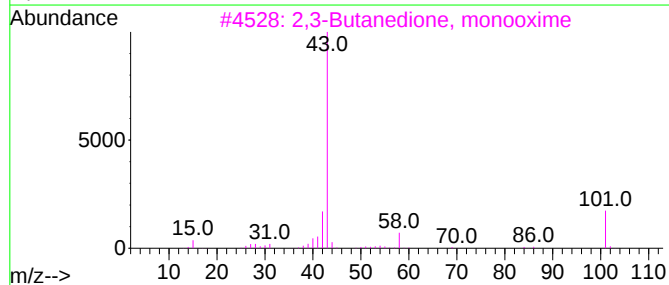
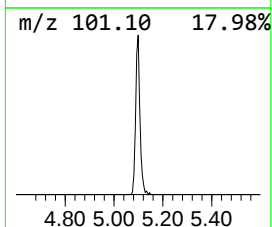
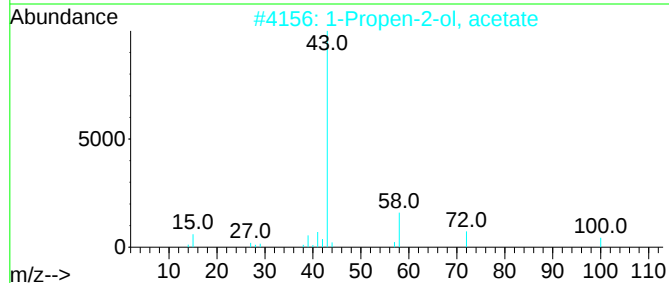
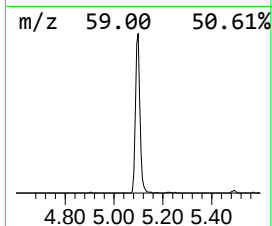
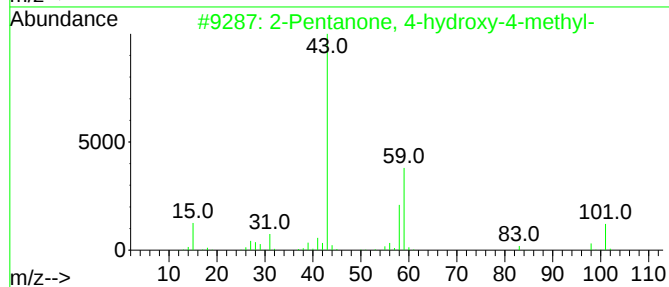
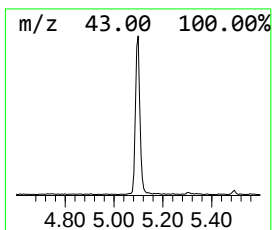
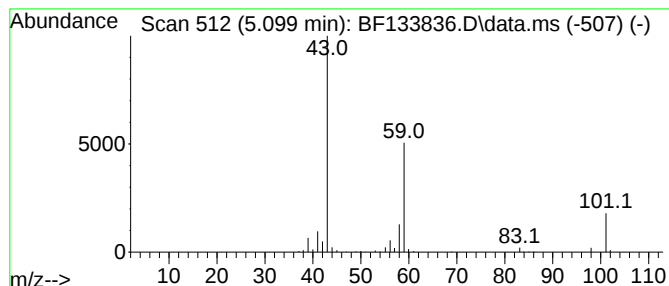
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	7.98 ng	237200	1,4-Dichlorobenzene-d4	6.857

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9



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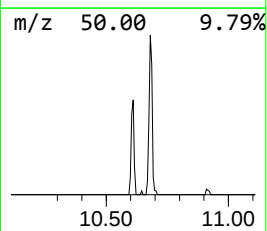
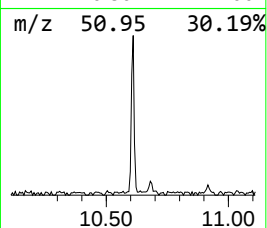
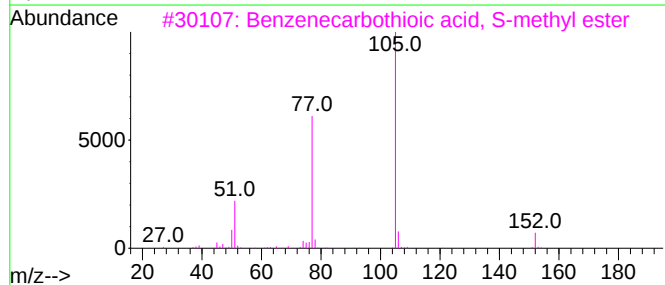
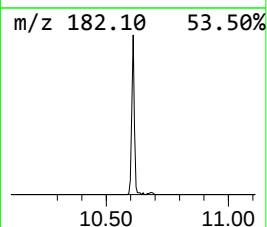
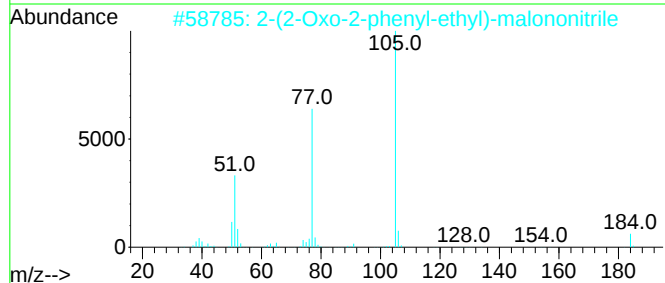
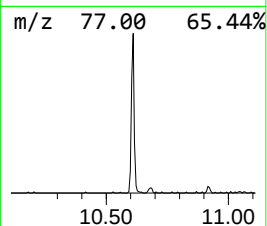
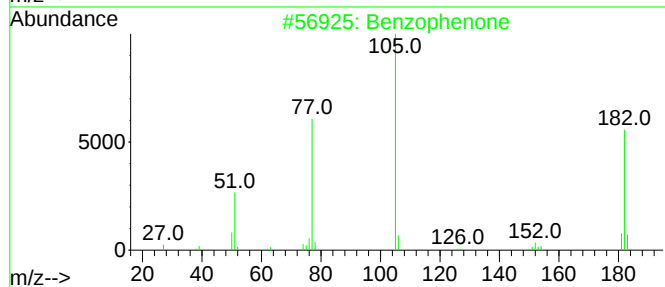
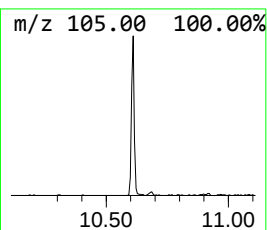
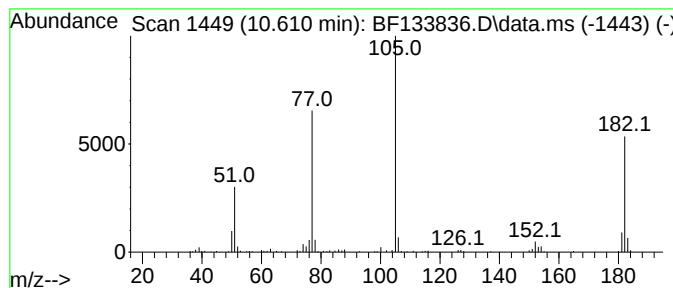
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	2.96 ng	118048	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	53
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	49
5			Benzoylformic acid	150	C8H6O3	000611-73-4	49



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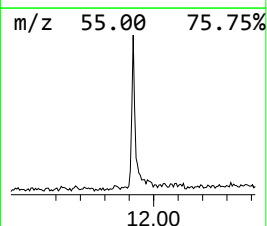
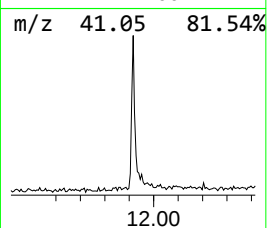
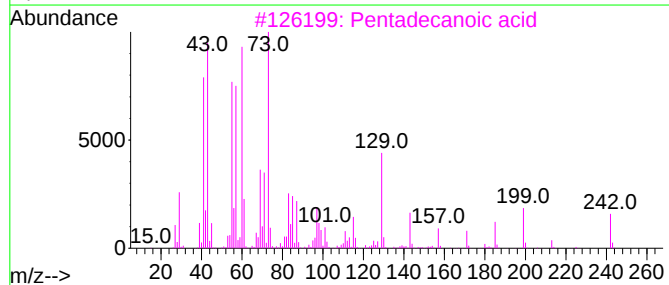
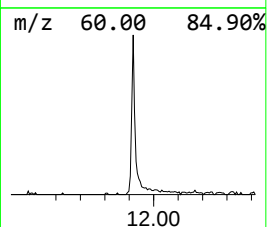
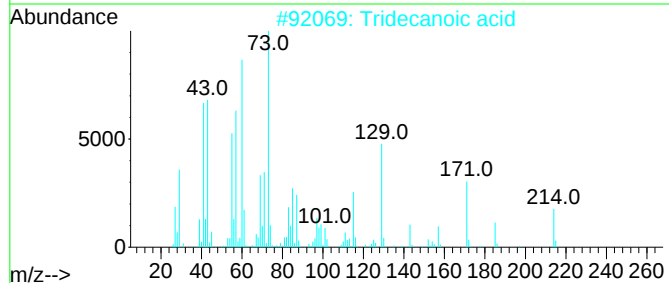
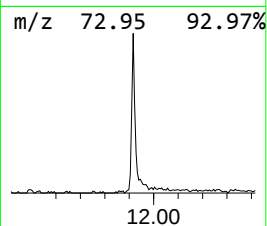
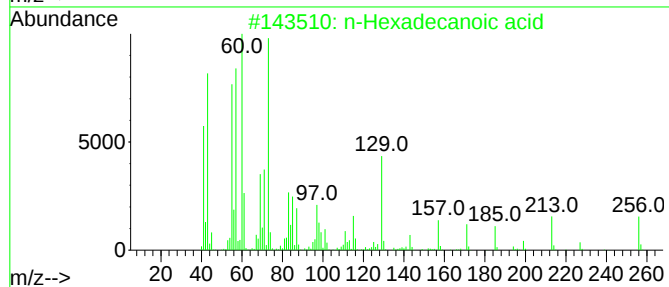
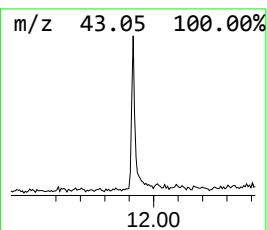
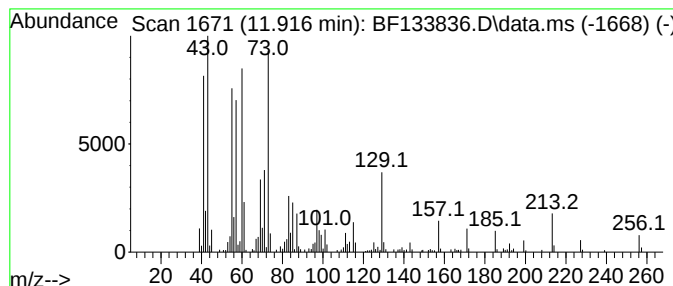
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	5.70 ng	210705	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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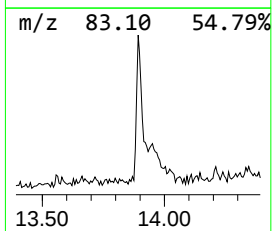
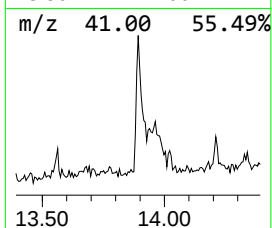
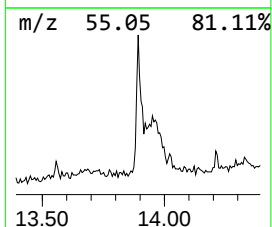
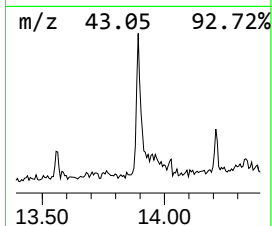
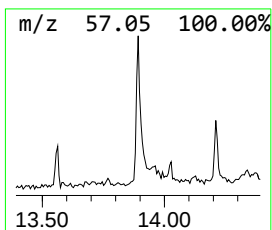
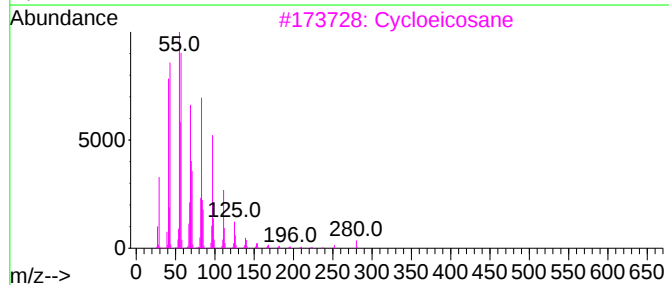
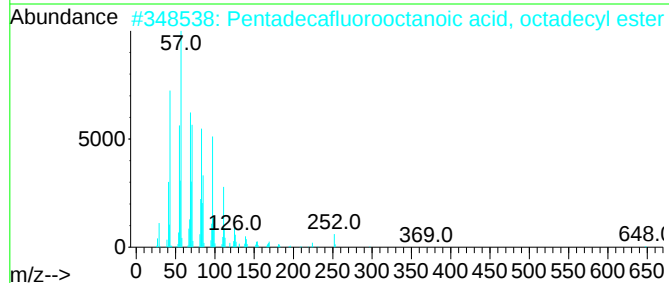
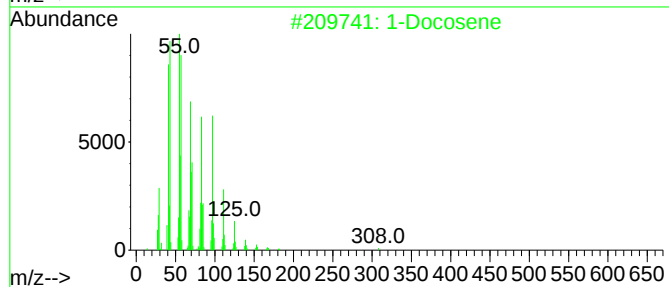
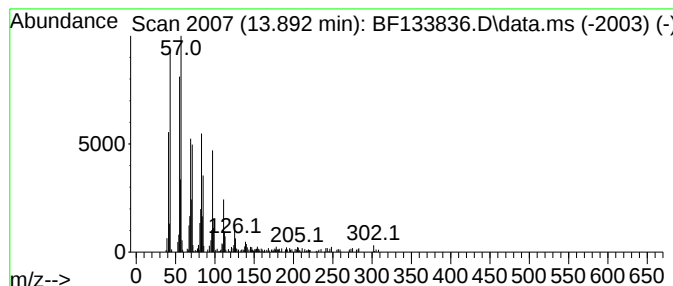
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	7.67 ng	240447	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	99
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
3			Cycloeicosane	280	C20H40	000296-56-0	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91



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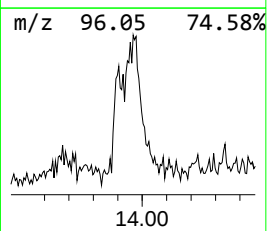
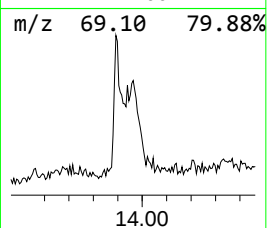
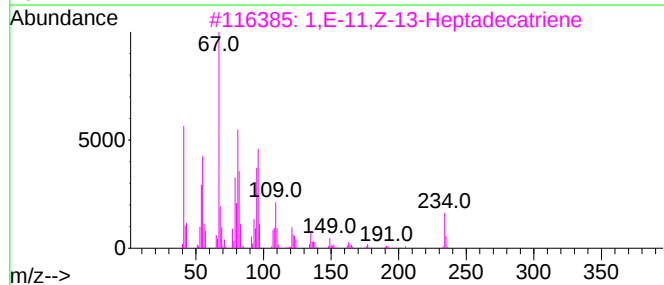
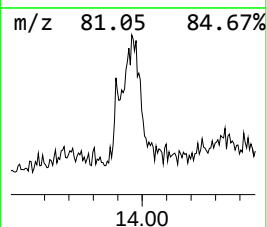
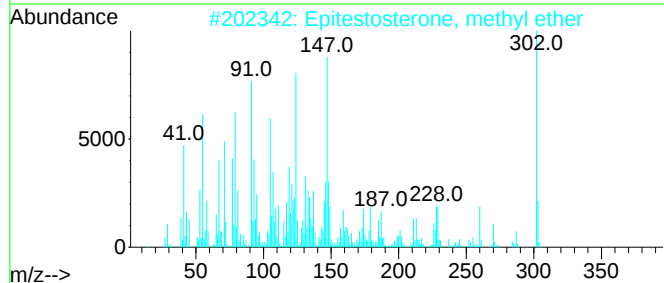
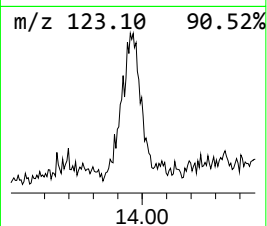
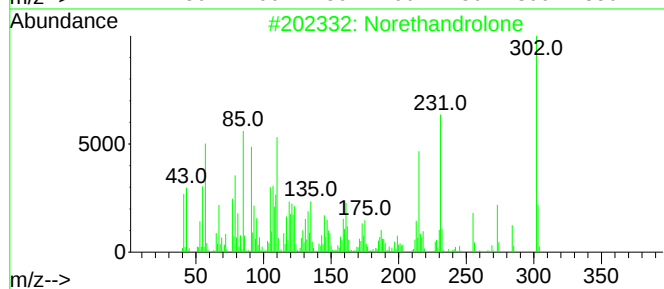
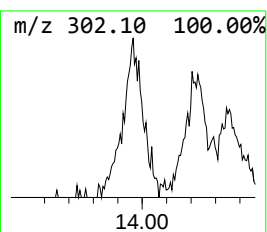
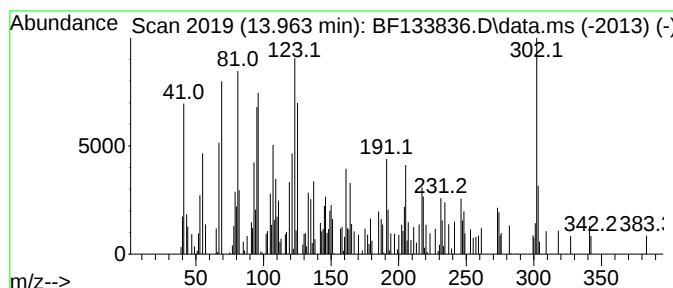
Instrument :
BNA_F
ClientSampleId :
WC-NEX-001

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 6 unknown13.963 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.963	11.41 ng	357730	Chrysene-d12		14.045	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Norethandrolone		302	C20H30O2	000052-78-8	38
2	Epitestosterone, methyl ether		302	C20H30O2	1000332-94-3	25
3	1,E-11,Z-13-Heptadecatriene		234	C17H30	080625-35-0	25
4	Aristolene epoxide		220	C15H24O	1000151-48-9	25
5	1,2,9,10-Dibenzopyrene		302	C24H14	000191-30-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061923\
Data File : BF133836.D
Acq On : 19 Jun 2023 16:31
Operator : CG\JU
Sample : 03282-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-NEX-001

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
Butane, 2-metho...	2.158	24.7	ng	735713	1	6.857	594793	20.0
2-Pentanone, 4-...	5.099	8.0	ng	237200	1	6.857	594793	20.0
Benzophenone	10.610	3.0	ng	118048	3	9.892	796982	20.0
n-Hexadecanoic ...	11.916	5.7	ng	210705	4	11.386	739094	20.0
1-Docosene	13.892	7.7	ng	240447	5	14.045	627104	20.0
unknown13.963	13.963	11.4	ng	357730	5	14.045	627104	20.0