

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
 Data File : BF131601.D
 Acq On : 12 Dec 2022 19:44
 Operator : CG\JU
 Sample : N5964-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-518-COMP-02

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: BF131601.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	14	22	rVB	424572	522210	30.55%	4.132%
2	2.275	28	32	39	rBV	22405	28584	1.67%	0.226%
3	2.499	65	70	77	rVB2	11775	21908	1.28%	0.173%
4	5.104	509	513	521	rVB	176937	214367	12.54%	1.696%
5	5.510	577	582	585	rBV	1612860	1485720	86.92%	11.756%
6	6.522	749	754	757	rBV	1503687	1515261	88.65%	11.990%
7	6.892	813	817	820	rBV	421661	349652	20.46%	2.767%
8	7.457	908	913	916	rBV	1086521	966464	56.54%	7.648%
9	8.181	1031	1036	1039	rBV	534786	442333	25.88%	3.500%
10	9.263	1214	1220	1223	rBV	2095630	1709260	100.00%	13.525%
11	9.945	1332	1336	1339	rBV	647765	517385	30.27%	4.094%
12	10.739	1467	1471	1474	rBV	1329407	1099147	64.31%	8.697%
13	11.445	1587	1591	1593	rBV	559310	528609	30.93%	4.183%
14	11.463	1593	1594	1598	rVV	158133	114966	6.73%	0.910%
15	11.516	1598	1603	1606	rVB	43242	44397	2.60%	0.351%
16	11.969	1678	1680	1684	rVB2	71691	56512	3.31%	0.447%
17	12.057	1692	1695	1697	rBV	20594	21974	1.29%	0.174%
18	12.221	1718	1723	1725	rBV2	23389	20624	1.21%	0.163%
19	12.663	1794	1798	1801	rBV	189318	164378	9.62%	1.301%
20	12.892	1834	1837	1842	rVB	164549	138553	8.11%	1.096%
21	13.039	1858	1862	1865	rVB	1540961	1346783	78.79%	10.657%
22	13.604	1954	1958	1963	rBV	27737	32530	1.90%	0.257%
23	13.939	2012	2015	2018	rBV	43643	37533	2.20%	0.297%
24	13.992	2018	2024	2034	rVV6	25790	88158	5.16%	0.698%
25	14.098	2037	2042	2044	rVV2	378045	389280	22.77%	3.080%
26	14.121	2044	2046	2052	rVB	69402	62771	3.67%	0.497%
27	14.192	2053	2058	2062	rBV	59612	61326	3.59%	0.485%
28	14.257	2065	2069	2072	rBV	39876	38031	2.22%	0.301%
29	14.563	2116	2121	2127	rBV2	37674	40191	2.35%	0.318%
30	14.880	2170	2175	2179	rBV2	26778	31502	1.84%	0.249%
31	15.157	2218	2222	2226	rBV	49269	77301	4.52%	0.612%
32	15.474	2272	2276	2283	rVB	26762	33046	1.93%	0.261%
33	15.539	2283	2287	2292	rVB	44332	53254	3.12%	0.421%
34	15.610	2293	2299	2303	rBV	245343	319932	18.72%	2.532%
35	17.133	2553	2558	2566	rVB5	16975	36090	2.11%	0.286%
36	17.598	2630	2637	2642	rVB	13914	27545	1.61%	0.218%

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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-BF120822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

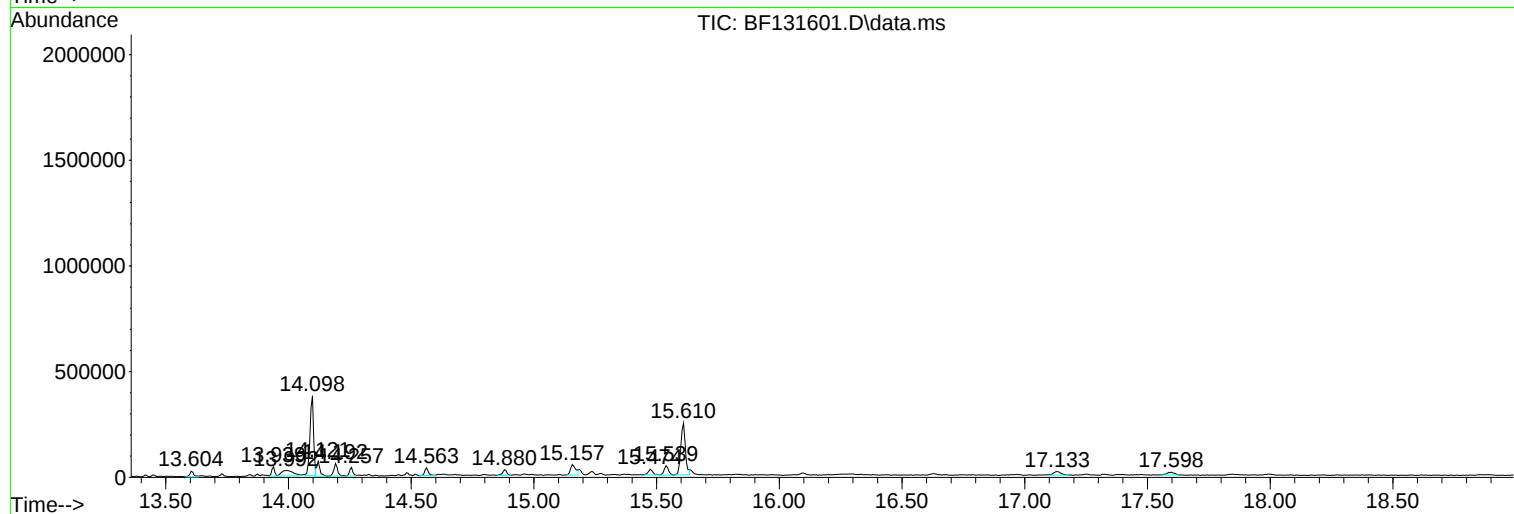
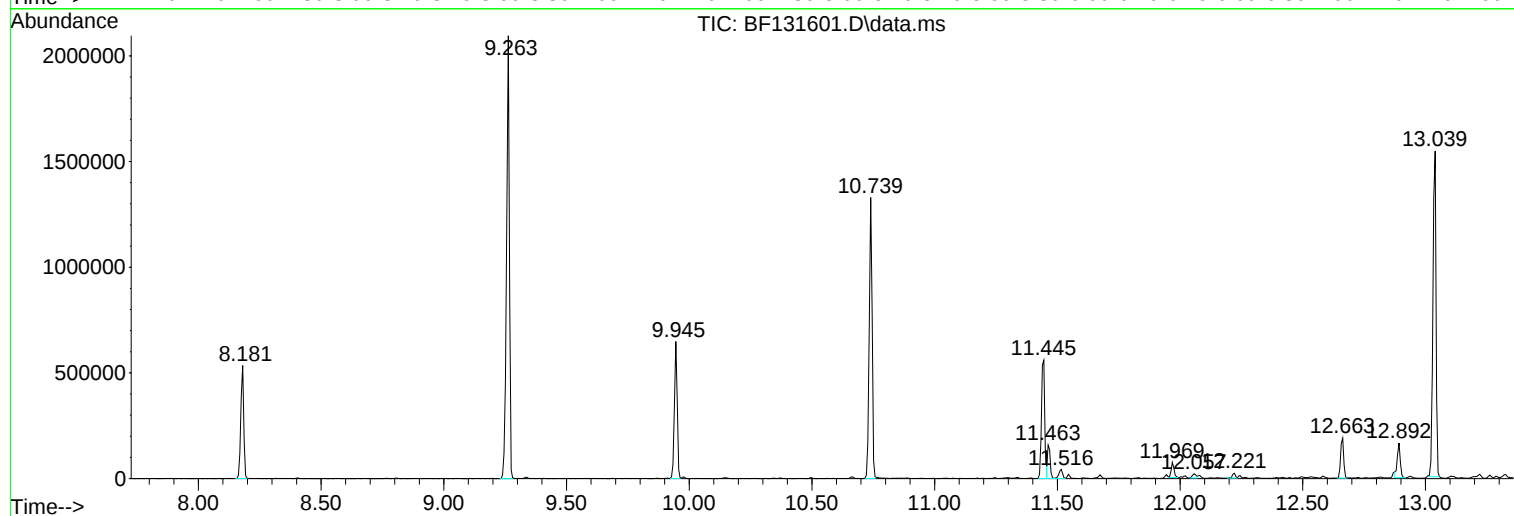
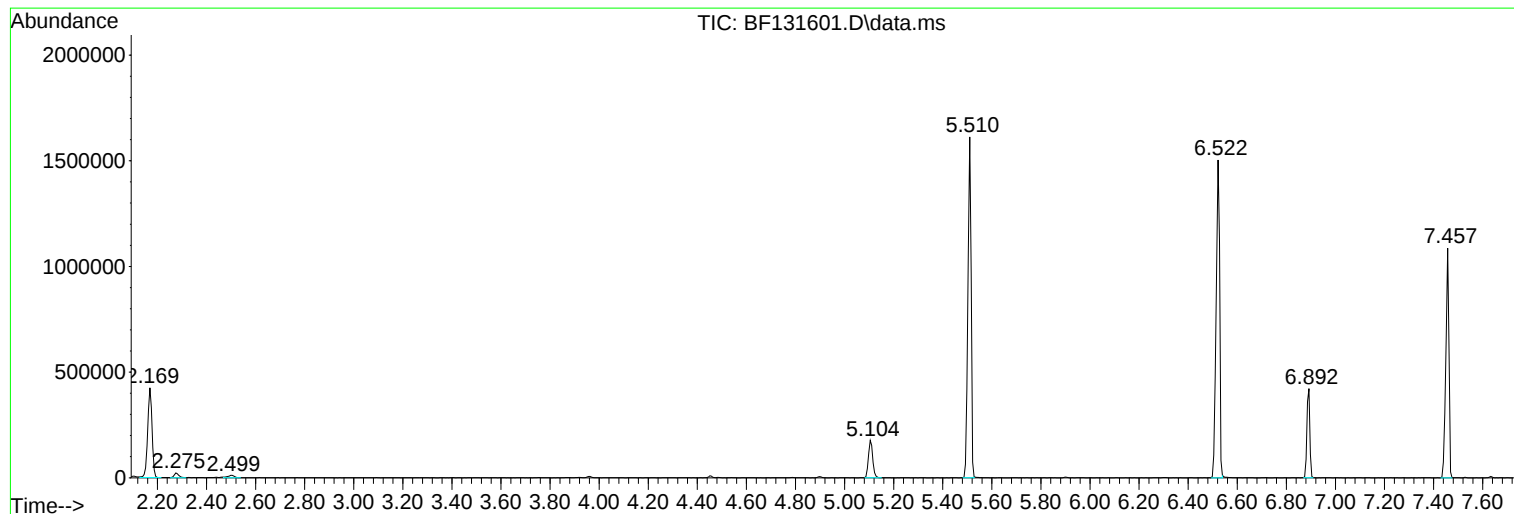
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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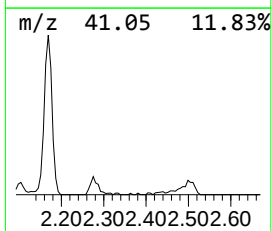
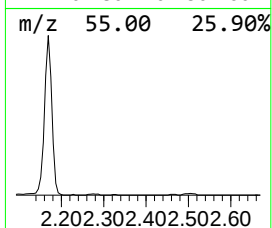
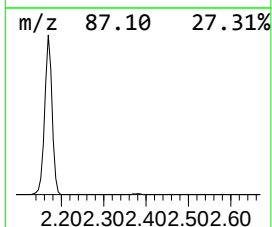
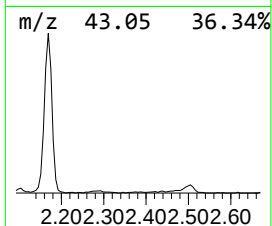
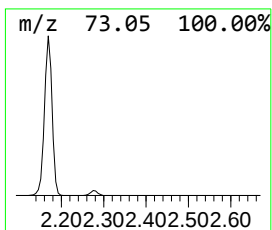
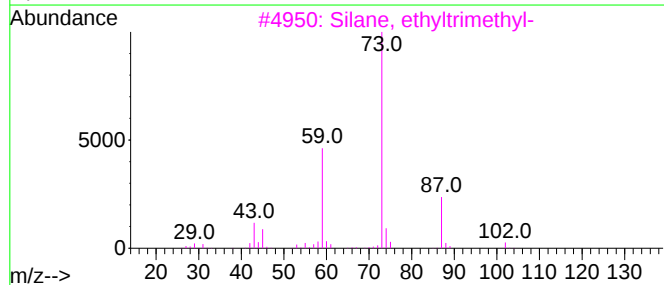
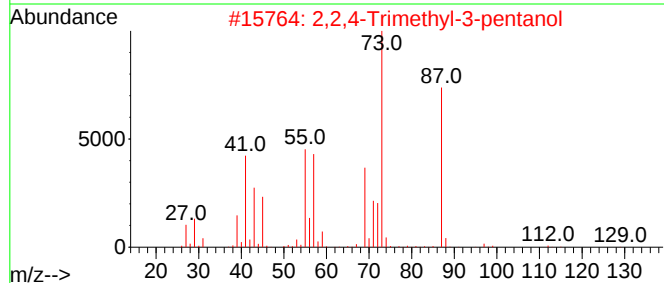
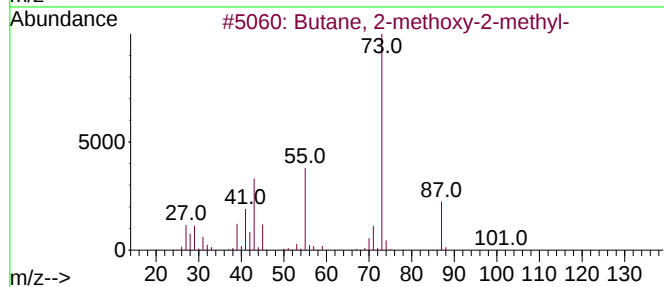
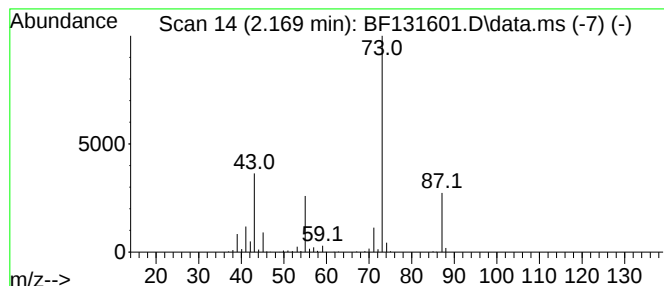
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	29.87 ng	522210	1,4-Dichlorobenzene-d4	6.892

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, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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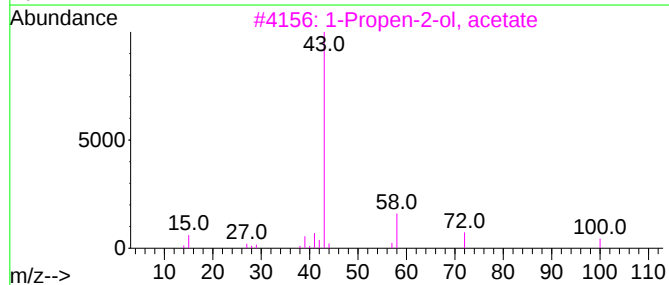
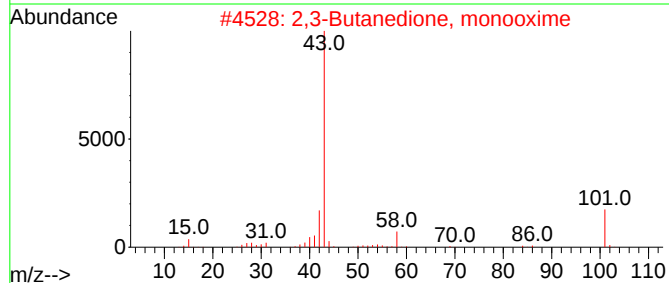
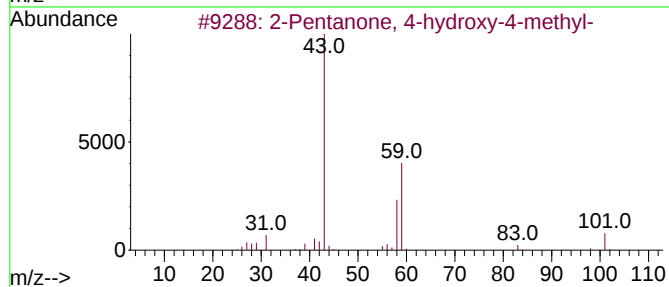
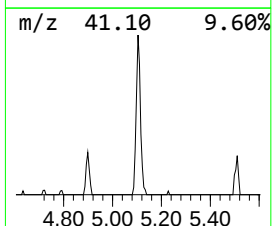
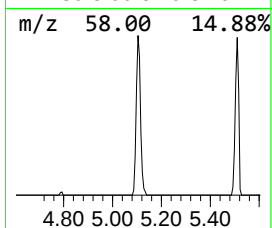
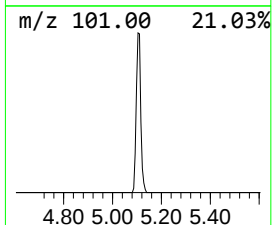
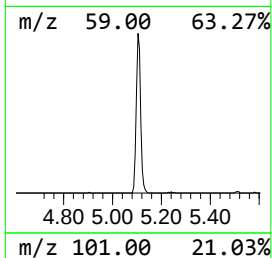
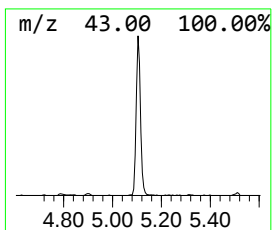
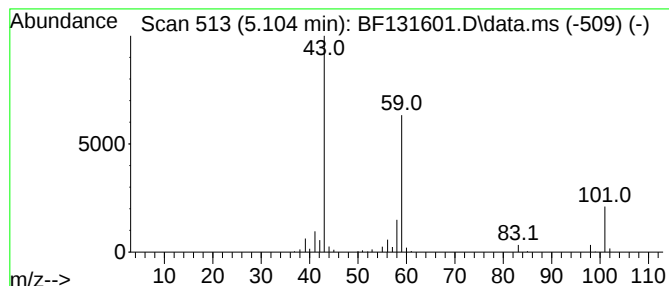
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	12.26 ng	214367	1,4-Dichlorobenzene-d4	6.892

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	12
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9



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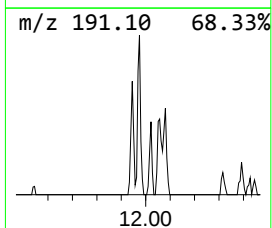
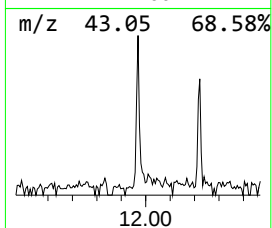
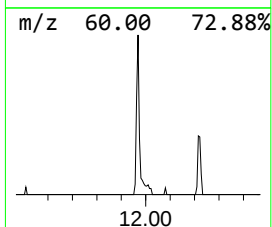
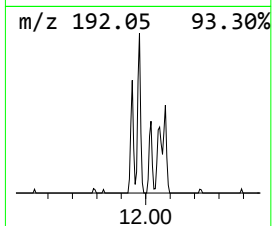
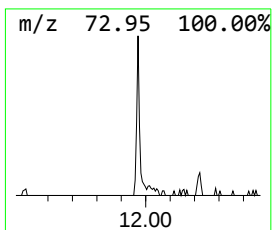
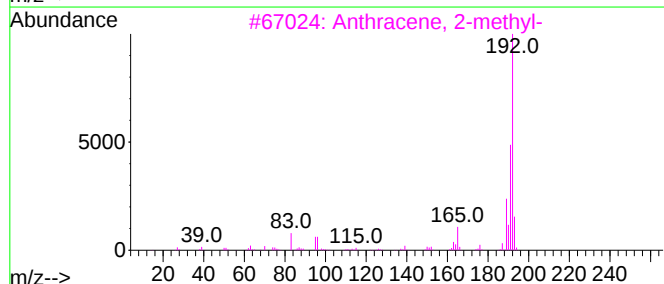
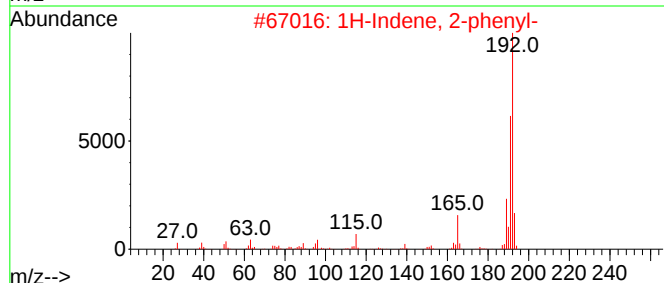
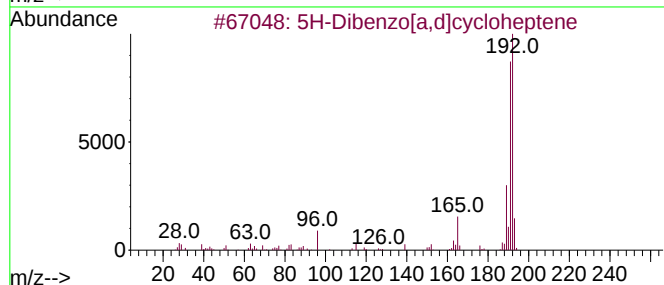
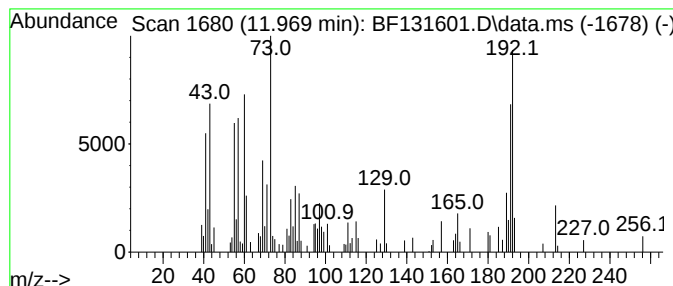
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown11.969 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	2.14 ng	56512	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	42
2			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	42
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	42
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42



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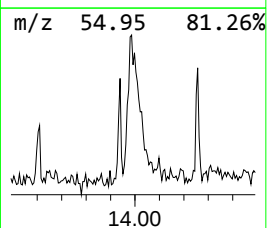
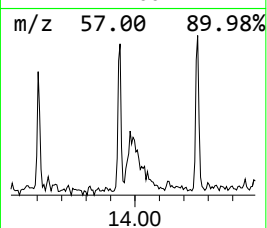
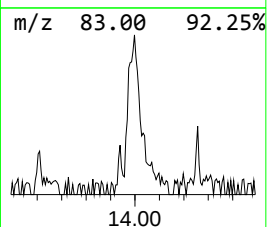
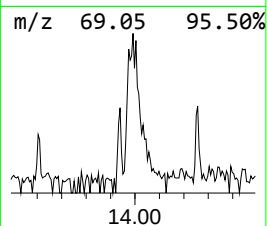
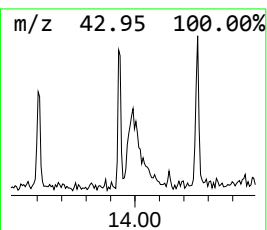
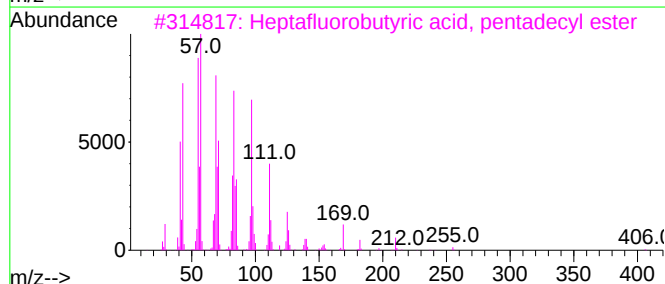
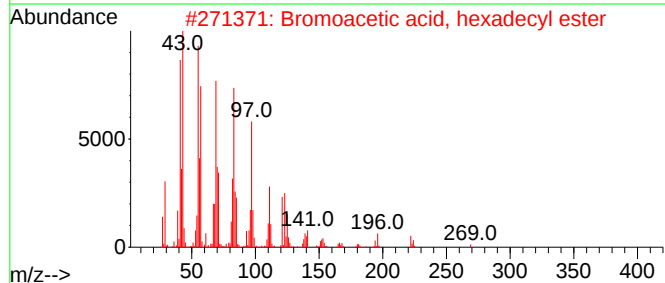
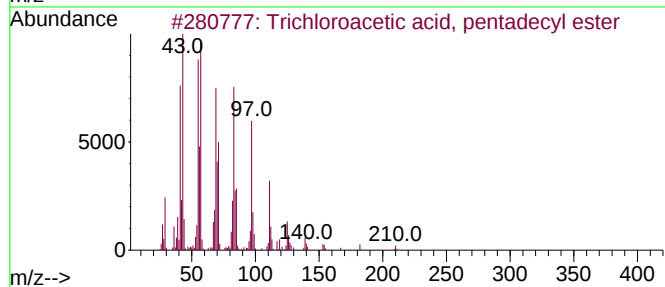
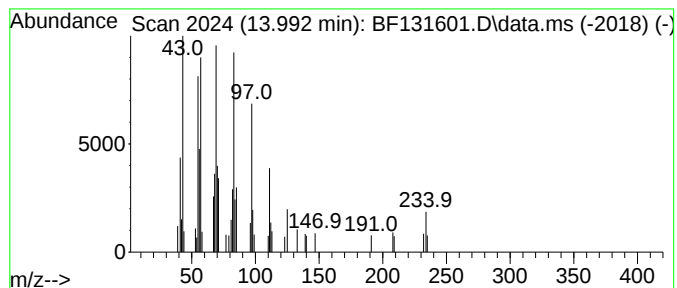
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Trichloroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	4.53 ng	88158	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
2			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	83
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	81
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	70



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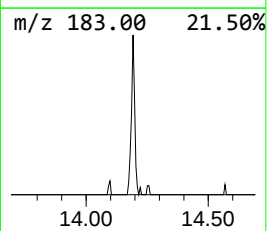
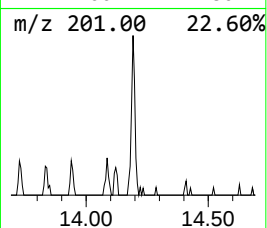
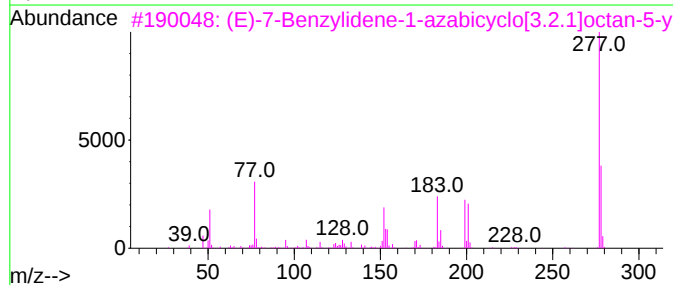
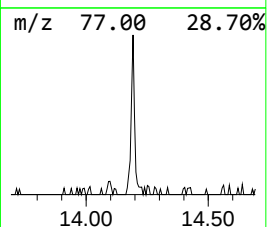
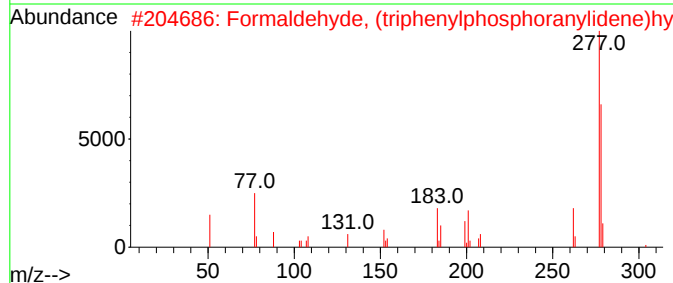
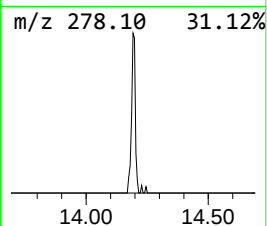
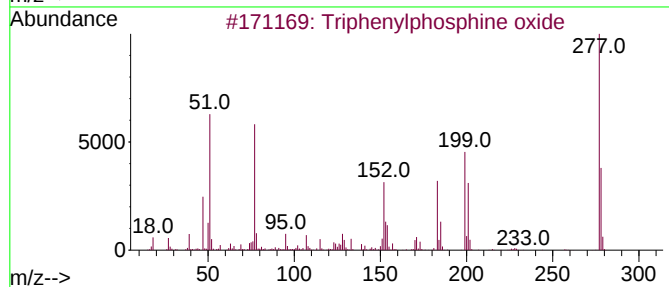
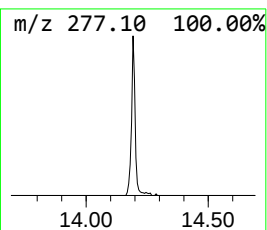
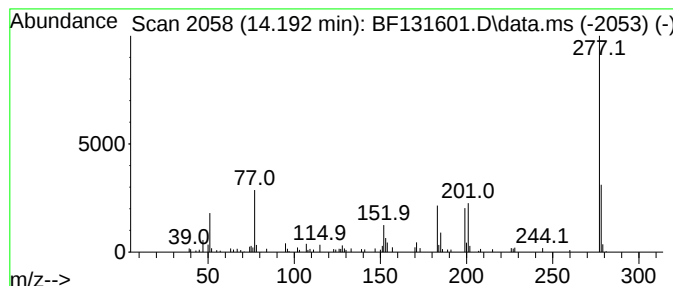
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	3.15 ng	61326	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	83
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	47
4			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	38
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131601.D
Acq On : 12 Dec 2022 19:44
Operator : CG\JU
Sample : N5964-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-518-COMP-02

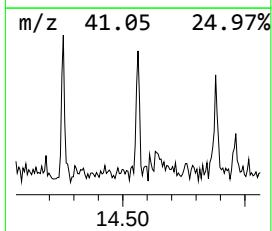
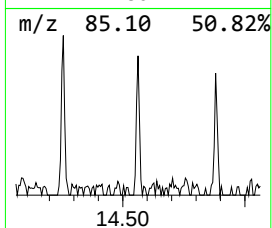
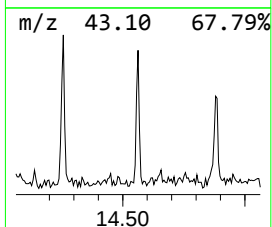
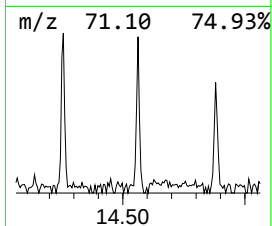
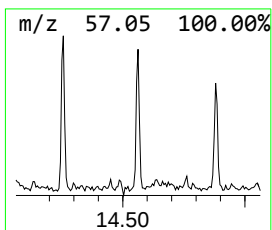
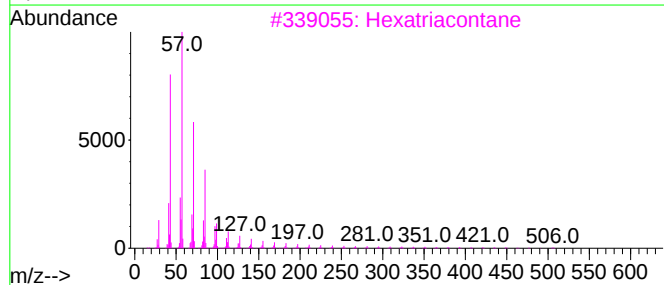
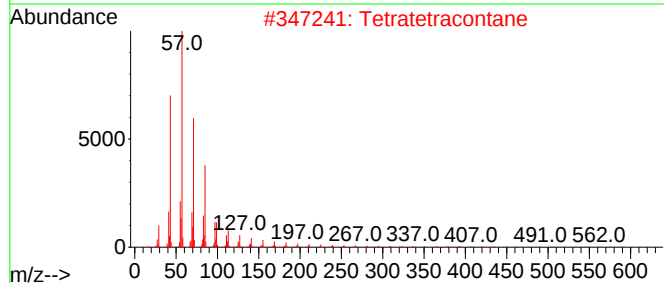
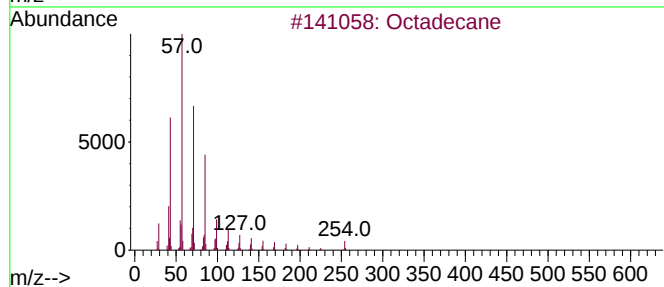
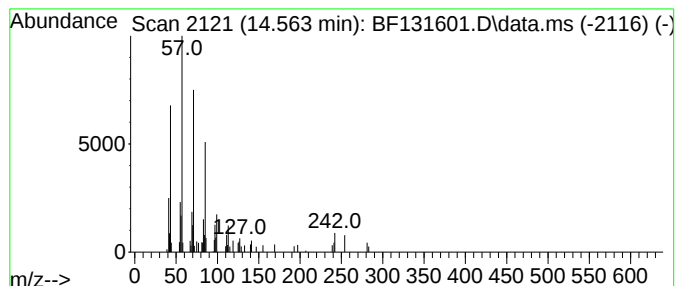
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.563	2.06 ng	40191	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	93
2			Tetratetracontane	619	C44H90	007098-22-8	90
3			Hexatriacontane	507	C36H74	000630-06-8	87
4			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131601.D
Acq On : 12 Dec 2022 19:44
Operator : CG\JU
Sample : N5964-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-518-COMP-02

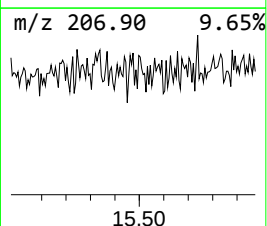
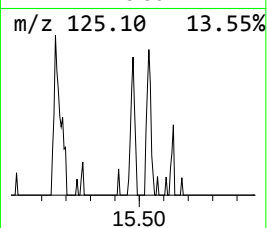
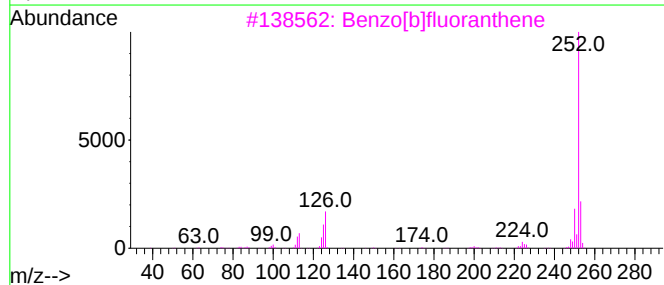
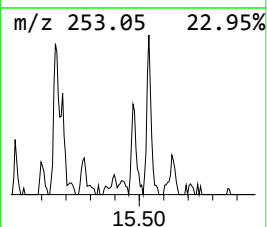
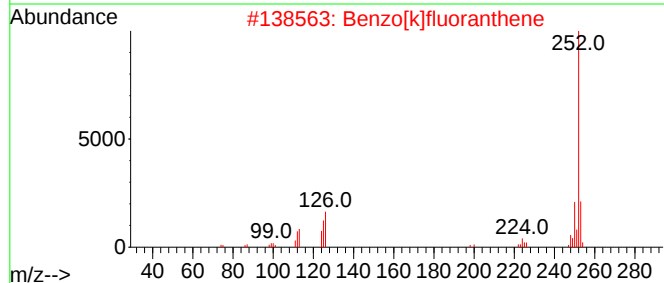
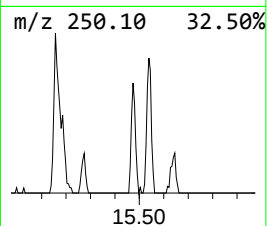
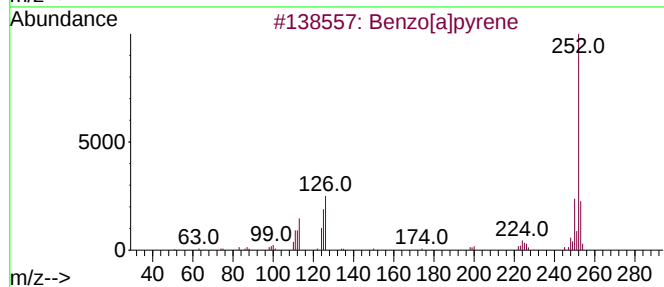
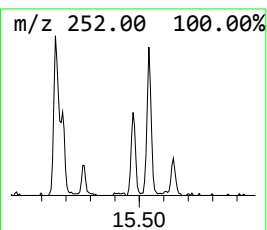
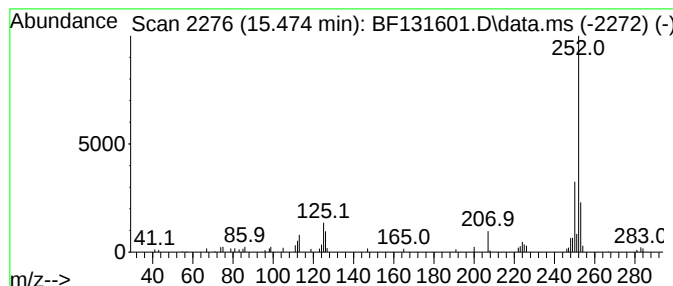
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.474	2.07 ng	33046	Perylene-d12	15.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	94
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	92
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	89
4			Benzo[e]pyrene	252	C20H12	000192-97-2	89
5			Perylene	252	C20H12	000198-55-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131601.D
Acq On : 12 Dec 2022 19:44
Operator : CG\JU
Sample : N5964-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-518-COMP-02

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...	2.169	29.9	ng	522210	1	6.892	349652	20.0
2-Pentanone, 4-...	5.104	12.3	ng	214367	1	6.892	349652	20.0
unknown11.969	11.969	2.1	ng	56512	4	11.445	528609	20.0
Trichloroacetic...	13.992	4.5	ng	88158	5	14.098	389280	20.0
Triphenylphosph...	14.192	3.1	ng	61326	5	14.098	389280	20.0
Octadecane	14.563	2.1	ng	40191	5	14.098	389280	20.0
Benzo[e]pyrene	15.474	2.1	ng	33046	6	15.610	319932	20.0