

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
 Data File : BF131656.D
 Acq On : 15 Dec 2022 18:57
 Operator : CG\JU
 Sample : N6038-09
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-33-(2-4)

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: BF131656.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	4	11	18	rVB	464747	561522	24.14%	3.174%
2	5.092	507	511	520	rVB	238756	304668	13.10%	1.722%
3	5.498	575	580	583	rBV	2270934	2089305	89.81%	11.810%
4	6.510	747	752	755	rBV	1904088	2152193	92.51%	12.166%
5	6.881	811	815	818	rVB	588457	454849	19.55%	2.571%
6	7.451	906	912	915	rBV	1387739	1390960	59.79%	7.863%
7	8.169	1029	1034	1037	rBV	700776	579714	24.92%	3.277%
8	9.251	1212	1218	1221	rBV	2796005	2326466	100.00%	13.151%
9	9.933	1323	1334	1337	rBV	811511	678947	29.18%	3.838%
10	10.651	1450	1456	1459	rBV	121802	99231	4.27%	0.561%
11	10.727	1464	1469	1472	rBV	1898144	1603730	68.93%	9.065%
12	11.427	1584	1588	1590	rBV	853609	709443	30.49%	4.010%
13	11.451	1590	1592	1595	rVB	116975	89089	3.83%	0.504%
14	11.527	1603	1605	1609	rBV2	40127	33303	1.43%	0.188%
15	11.957	1675	1678	1681	rBV	114212	103931	4.47%	0.587%
16	12.039	1689	1692	1695	rBV2	37257	42475	1.83%	0.240%
17	12.480	1763	1767	1770	rBV	28208	29526	1.27%	0.167%
18	12.563	1779	1781	1786	rVB3	29574	30584	1.31%	0.173%
19	12.645	1791	1795	1798	rBV	322128	271196	11.66%	1.533%
20	12.874	1828	1834	1840	rVB	281424	268391	11.54%	1.517%
21	13.021	1855	1859	1862	rVV	2161234	1851973	79.60%	10.469%
22	13.092	1865	1871	1875	rBV3	23818	40031	1.72%	0.226%
23	13.174	1882	1885	1888	rBV3	20100	30207	1.30%	0.171%
24	13.204	1888	1890	1893	rVB	35726	30223	1.30%	0.171%
25	13.304	1904	1907	1911	rVB2	31294	32991	1.42%	0.186%
26	13.710	1969	1976	1981	rBV2	23612	34275	1.47%	0.194%
27	13.921	2009	2012	2031	rBV8	50722	200772	8.63%	1.135%
28	14.074	2031	2038	2041	rVV2	466649	562617	24.18%	3.180%
29	14.104	2041	2043	2045	rVV	114372	95263	4.09%	0.538%
30	14.174	2049	2055	2059	rBV2	44239	57959	2.49%	0.328%
31	14.233	2059	2065	2070	rVB5	21039	28971	1.25%	0.164%
32	14.462	2099	2104	2108	rVB	23828	27949	1.20%	0.158%
33	15.133	2214	2218	2222	rBV	86386	139485	6.00%	0.788%
34	15.451	2267	2272	2278	rVB	55110	80287	3.45%	0.454%
35	15.515	2278	2283	2289	rBV	84818	104537	4.49%	0.591%
36	15.580	2289	2294	2298	rBV	313518	406204	17.46%	2.296%

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RB-33-(2-4)

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

37	17.092	2545	2551	2559	rVB3	40600	84996	3.65%	0.480%
38	17.550	2623	2629	2636	rBV2	30769	62533	2.69%	0.353%

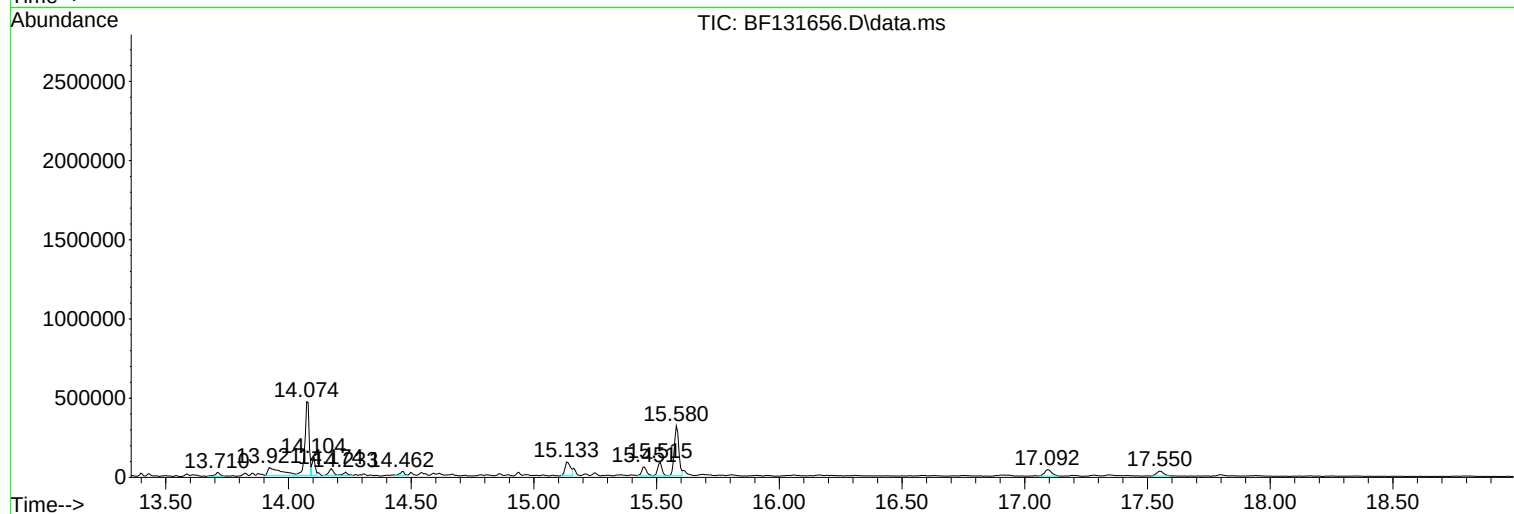
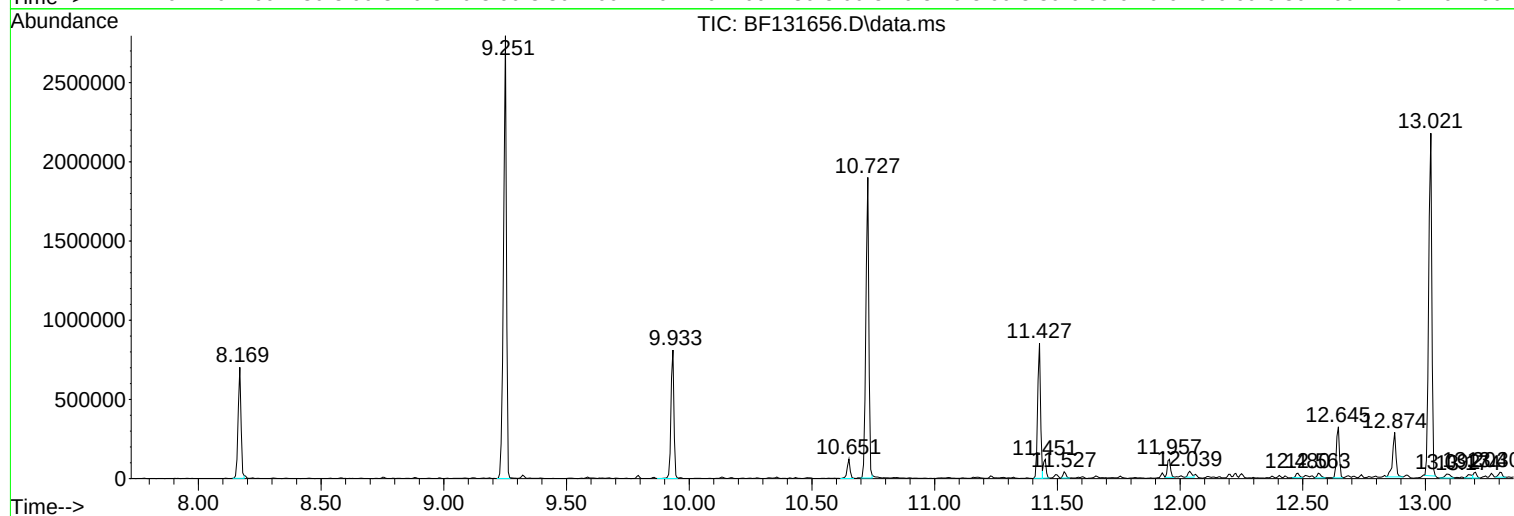
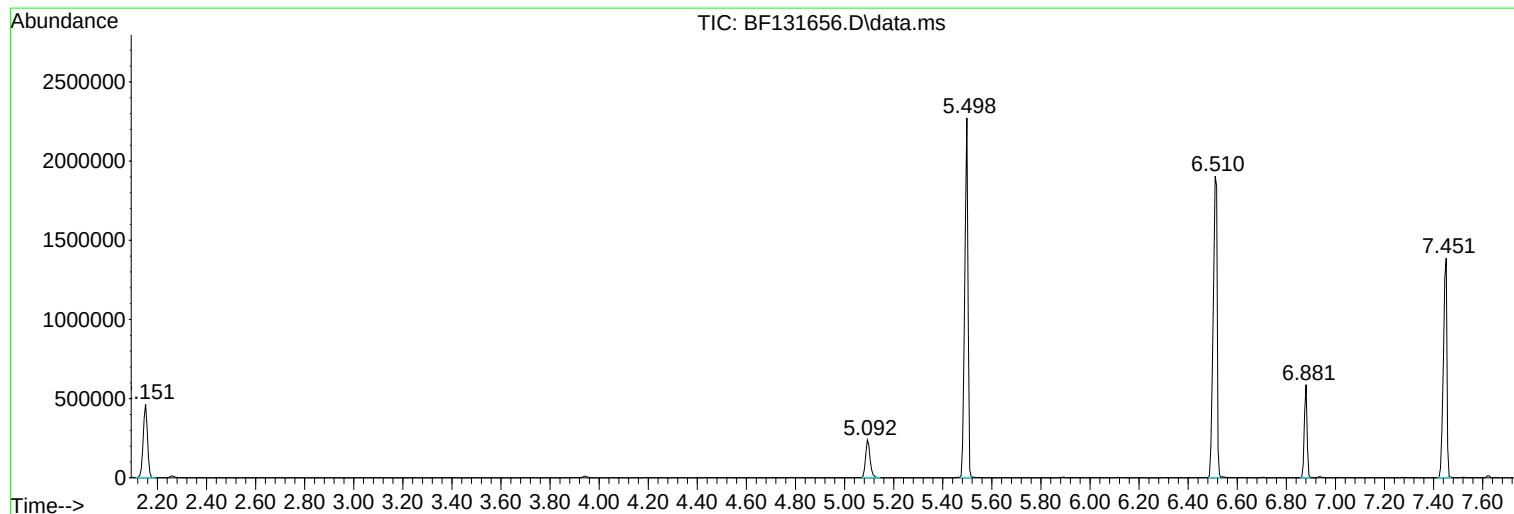
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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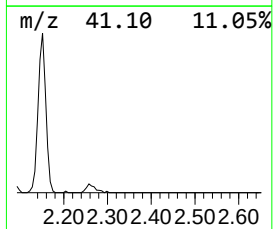
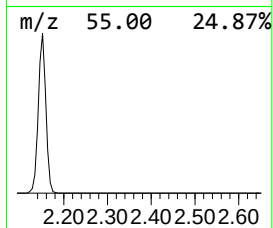
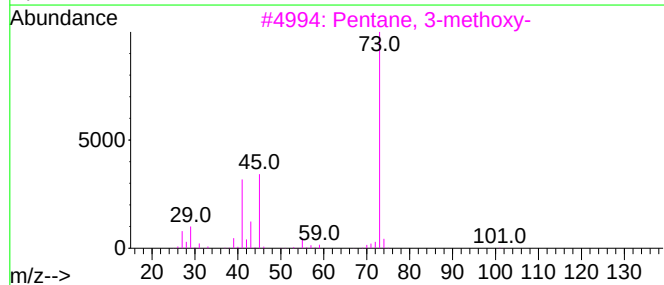
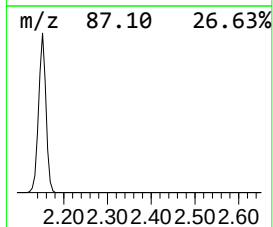
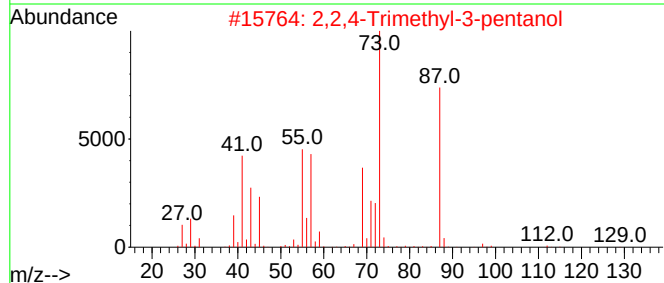
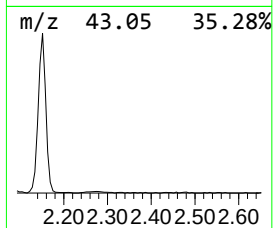
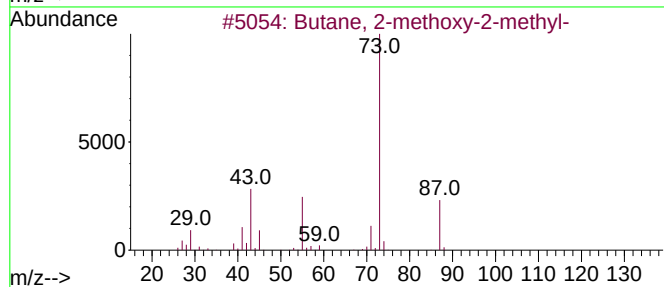
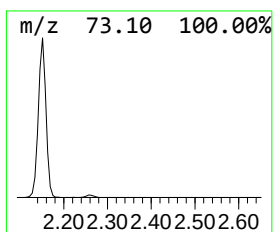
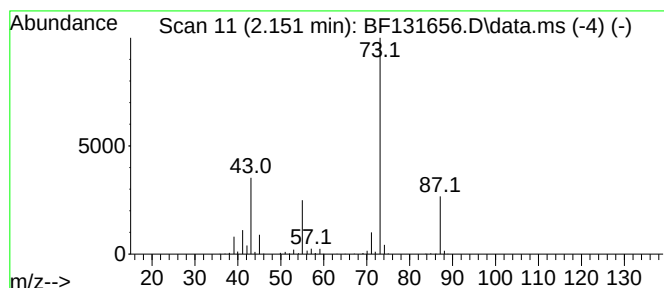
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.151	24.69 ng	561522	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	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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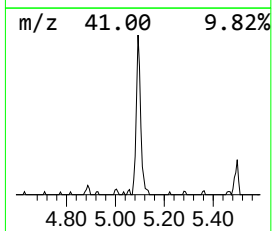
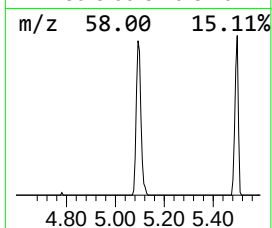
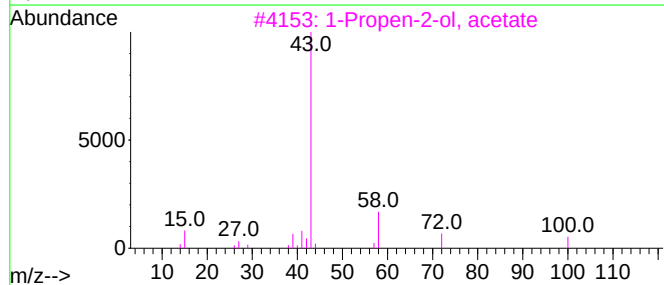
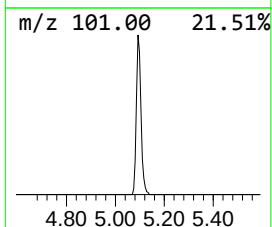
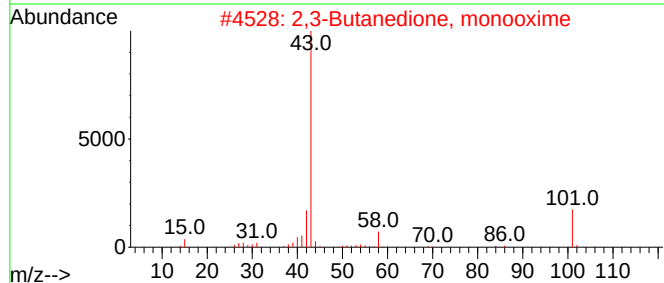
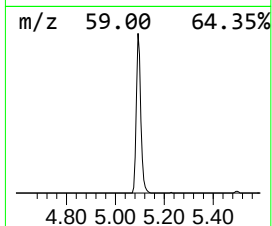
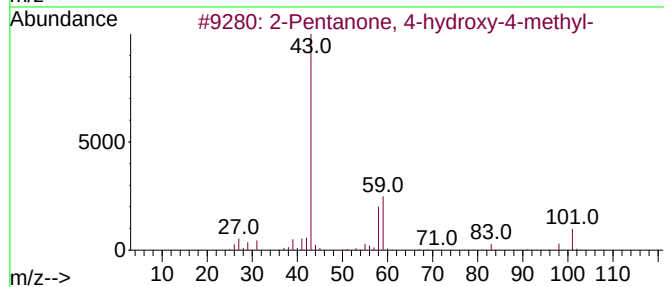
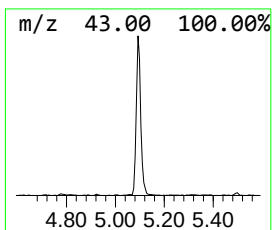
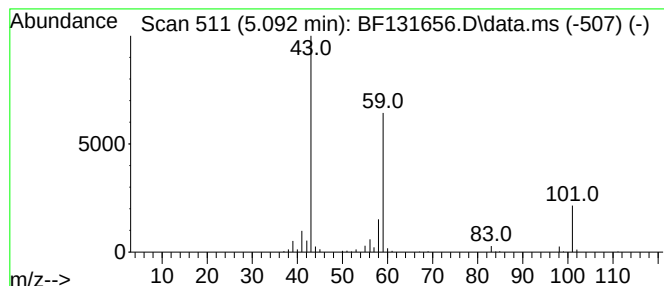
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	13.40 ng	304668	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	72
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9



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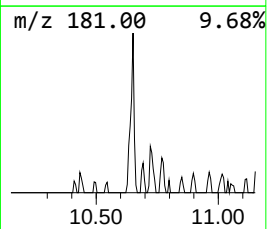
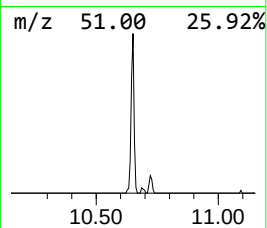
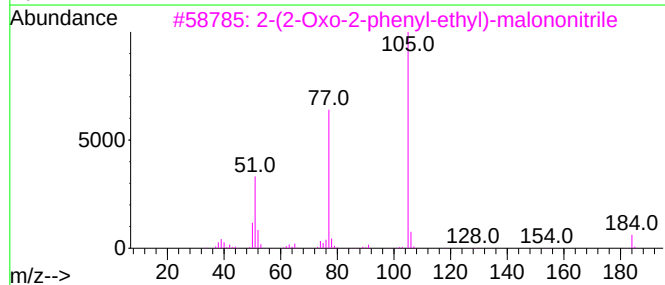
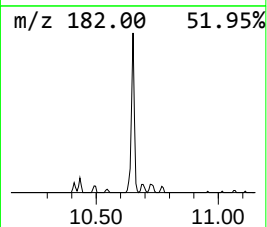
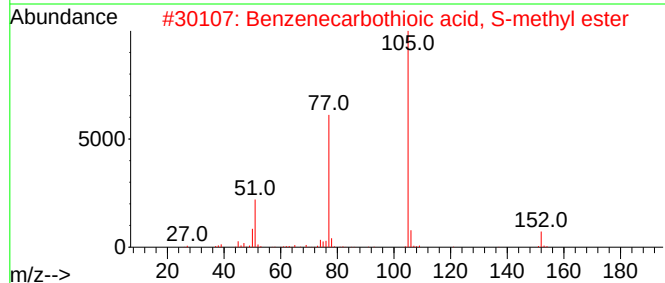
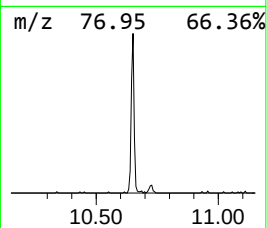
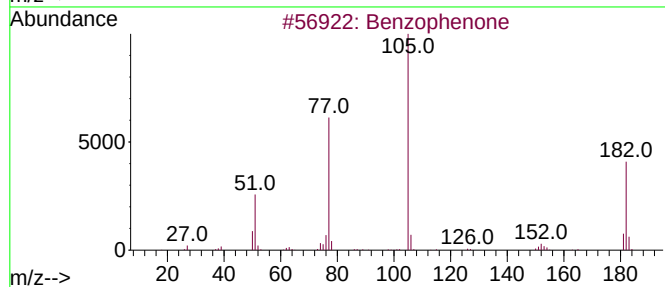
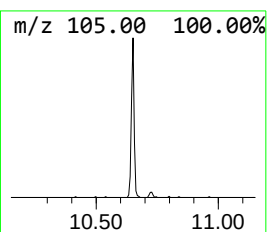
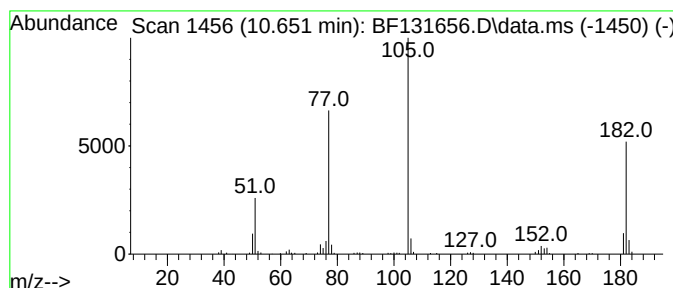
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	2.92 ng	99231	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
4			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
5			Methyl benzilate	242	C15H14O3	000076-89-1	47



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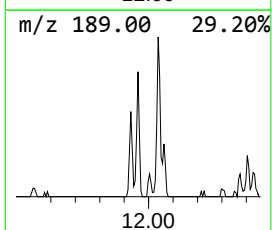
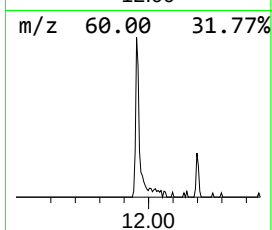
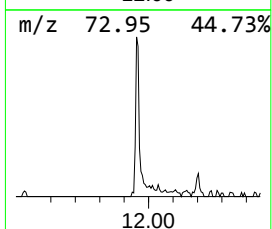
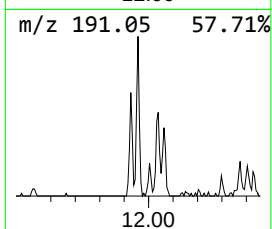
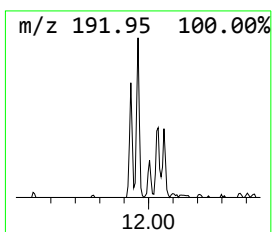
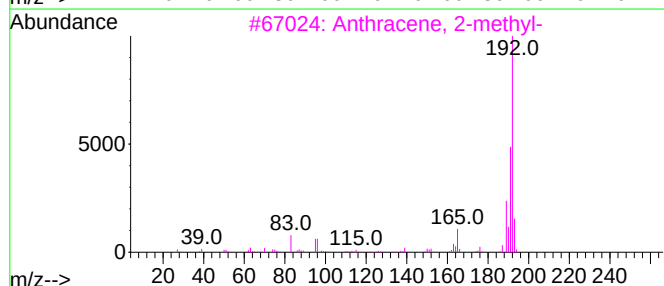
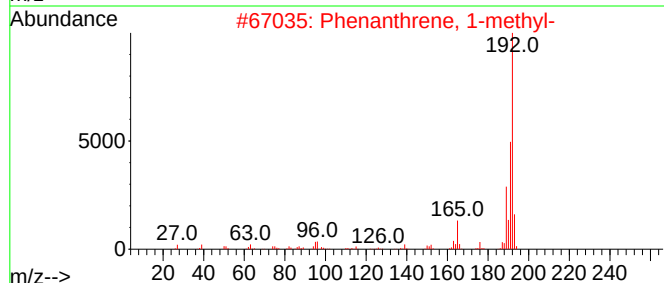
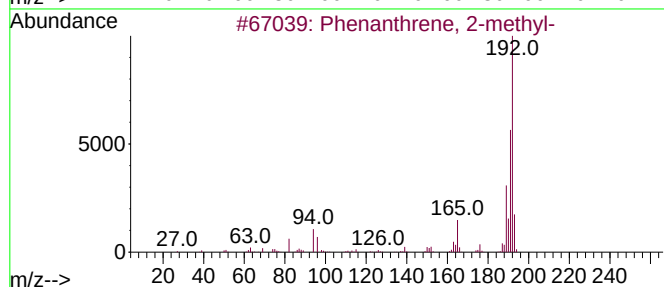
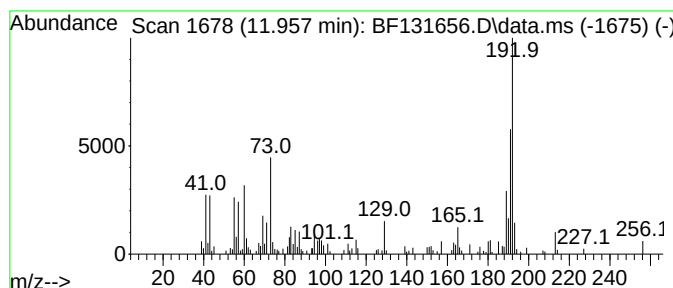
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	2.93 ng	103931	Phenanthrene-d10	11.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3		Anthracene, 2-methyl-	192	C15H12	000613-12-7	92
4		Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
5		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	91



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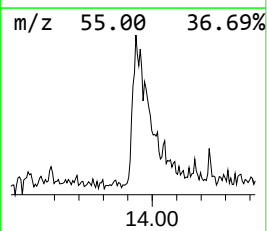
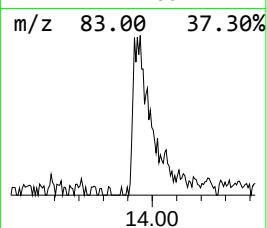
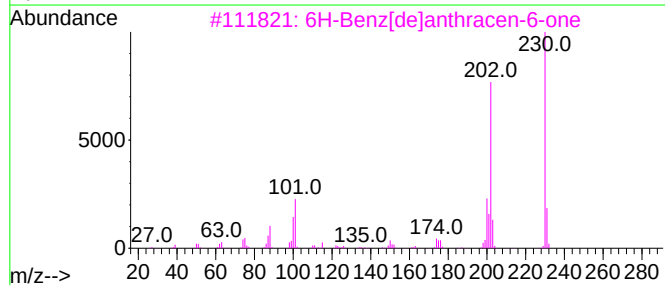
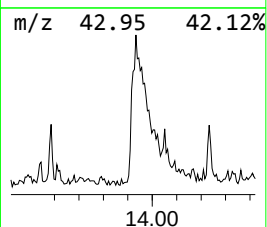
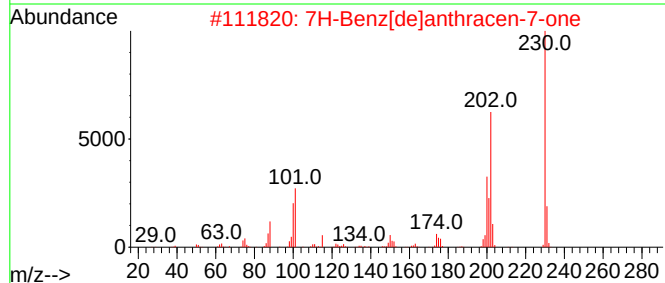
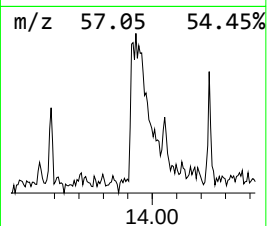
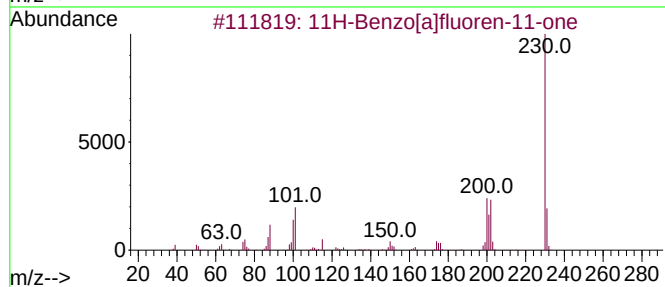
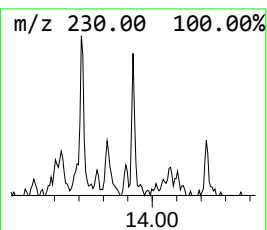
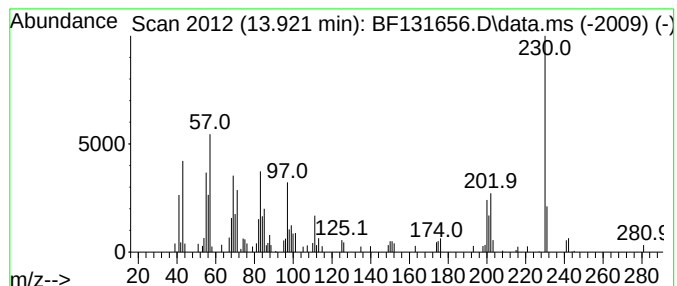
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 11H-Benzo[a]fluoren-11-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	7.14 ng	200772	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	86
2			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	58
3			6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	53
4			4,4'-Stilbenedicarbonitrile	230	C16H10N2	006292-62-2	46
5			(E)-.alpha.,.alpha.'-Dicyanostil...	230	C16H10N2	002450-55-7	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
Data File : BF131656.D
Acq On : 15 Dec 2022 18:57
Operator : CG\JU
Sample : N6038-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-33-(2-4)

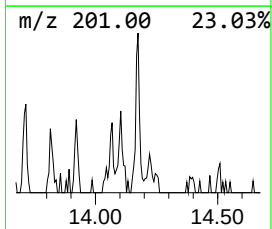
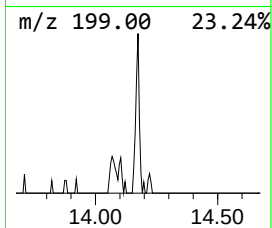
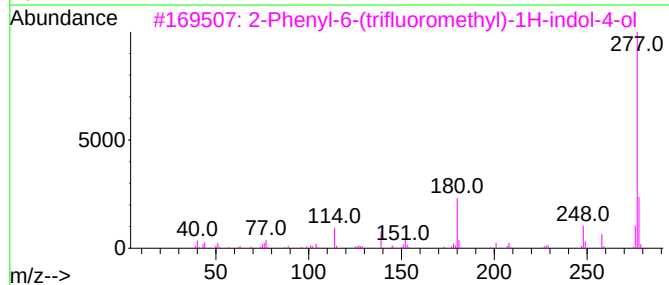
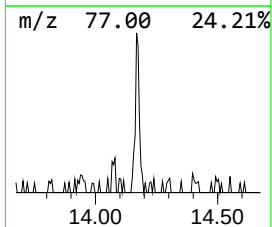
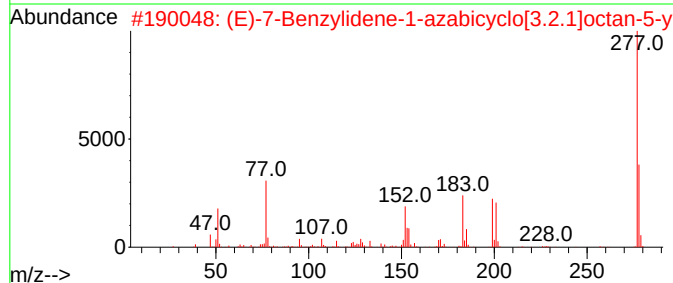
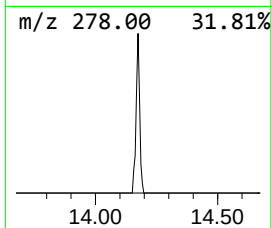
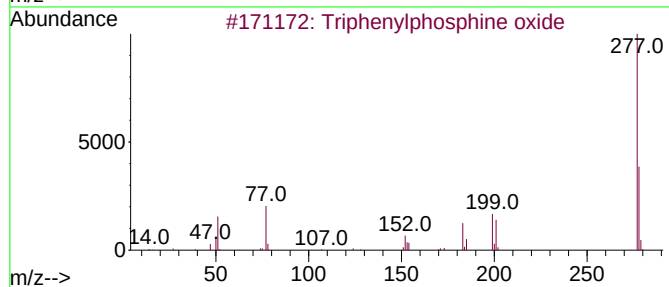
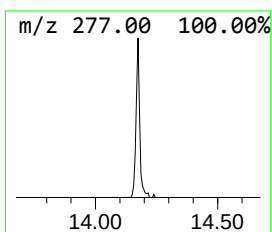
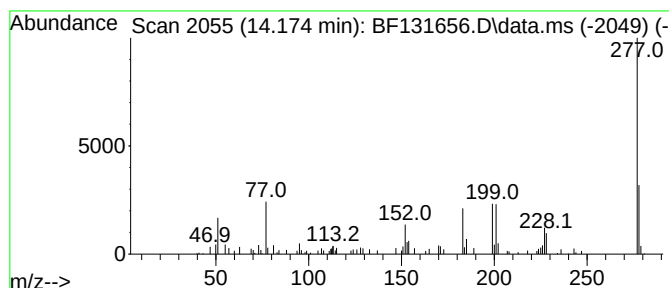
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.174	2.06 ng	57959	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	46
3			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	43
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
5			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
Data File : BF131656.D
Acq On : 15 Dec 2022 18:57
Operator : CG\JU
Sample : N6038-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-33-(2-4)

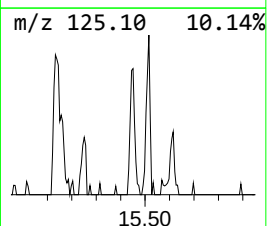
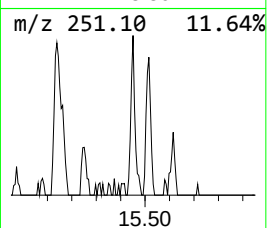
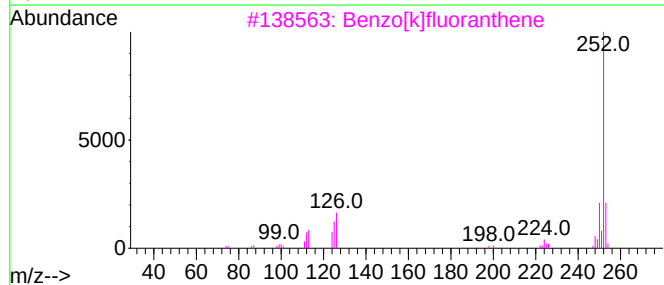
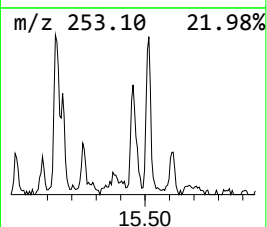
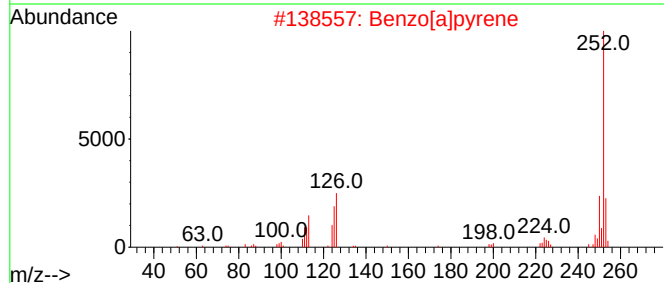
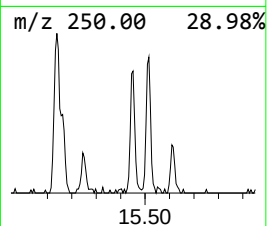
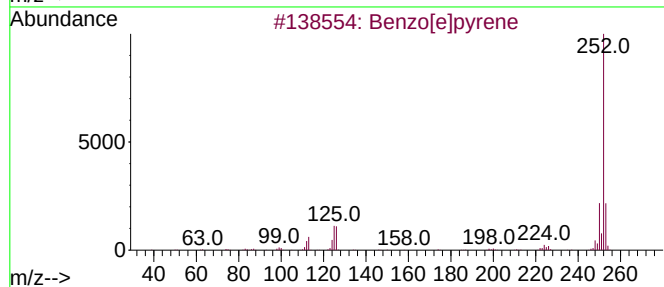
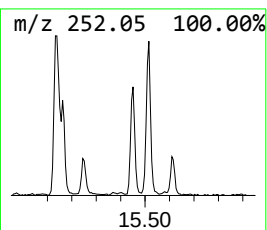
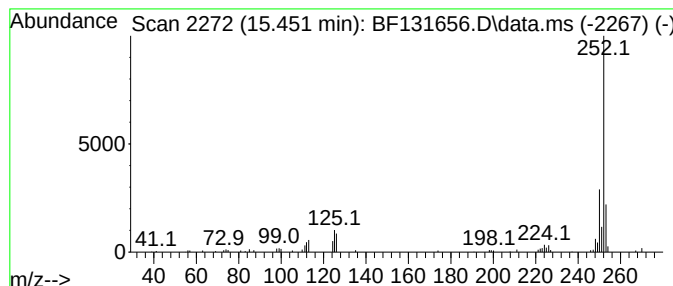
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.451	3.95 ng	80287	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[a]pyrene	252	C20H12	000050-32-8	97
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
5			Perylene	252	C20H12	000198-55-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
Data File : BF131656.D
Acq On : 15 Dec 2022 18:57
Operator : CG\JU
Sample : N6038-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-33-(2-4)

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...	2.151	24.7	ng	561522	1	6.881	454849	20.0
2-Pentanone, 4-...	5.092	13.4	ng	304668	1	6.881	454849	20.0
Benzophenone	10.651	2.9	ng	99231	3	9.933	678947	20.0
Phenanthrene, 2...	11.957	2.9	ng	103931	4	11.427	709443	20.0
11H-Benzo[a]flu...	13.921	7.1	ng	200772	5	14.080	562617	20.0
Triphenylphosph...	14.174	2.1	ng	57959	5	14.080	562617	20.0
Benzo[e]pyrene	15.451	4.0	ng	80287	6	15.580	406204	20.0