

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
 Data File : BF131139.D
 Acq On : 10 Nov 2022 23:44
 Operator : CG\JU
 Sample : N5494-17
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-20

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-BF110922.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131139.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	16	rBV	350717	428406	30.77%	4.165%
2	5.104	509	513	523	rBV	227977	247175	17.76%	2.403%
3	5.504	577	581	584	rBV	1596385	1392079	100.00%	13.534%
4	6.516	748	753	756	rBV	1495293	1325252	95.20%	12.885%
5	6.886	813	816	820	rVB	471001	362730	26.06%	3.527%
6	7.451	908	912	915	rBV	963588	828011	59.48%	8.050%
7	8.175	1031	1035	1038	rBV	515140	458915	32.97%	4.462%
8	9.245	1213	1217	1221	rBV	1408209	1223173	87.87%	11.892%
9	9.933	1330	1334	1337	rBV	476215	408948	29.38%	3.976%
10	10.721	1464	1468	1478	rBV	777207	647810	46.54%	6.298%
11	11.421	1584	1587	1591	rBV	452864	383339	27.54%	3.727%
12	12.639	1789	1794	1797	rVB	42858	38084	2.74%	0.370%
13	12.868	1828	1833	1837	rBV	46928	51885	3.73%	0.504%
14	13.010	1853	1857	1861	rBV	1278217	1118300	80.33%	10.873%
15	13.192	1882	1888	1892	rBV6	18262	30220	2.17%	0.294%
16	13.980	2015	2022	2031	rBV6	46431	156526	11.24%	1.522%
17	14.074	2033	2038	2041	rVV	562034	538301	38.67%	5.234%
18	14.098	2041	2042	2046	rVB	45228	28730	2.06%	0.279%
19	14.168	2050	2054	2058	rBV	54110	61782	4.44%	0.601%
20	14.221	2061	2063	2066	rBV	18467	16379	1.18%	0.159%
21	14.533	2113	2116	2118	rBV2	27177	25410	1.83%	0.247%
22	14.921	2179	2182	2188	rVB	31321	34750	2.50%	0.338%
23	15.127	2214	2217	2221	rBV	28522	40649	2.92%	0.395%
24	15.439	2268	2270	2275	rBV	17018	19811	1.42%	0.193%
25	15.504	2279	2281	2287	rVB	29020	36291	2.61%	0.353%
26	15.568	2288	2292	2301	rVB	243854	321357	23.08%	3.124%
27	17.168	2561	2564	2576	rVB	22023	61194	4.40%	0.595%

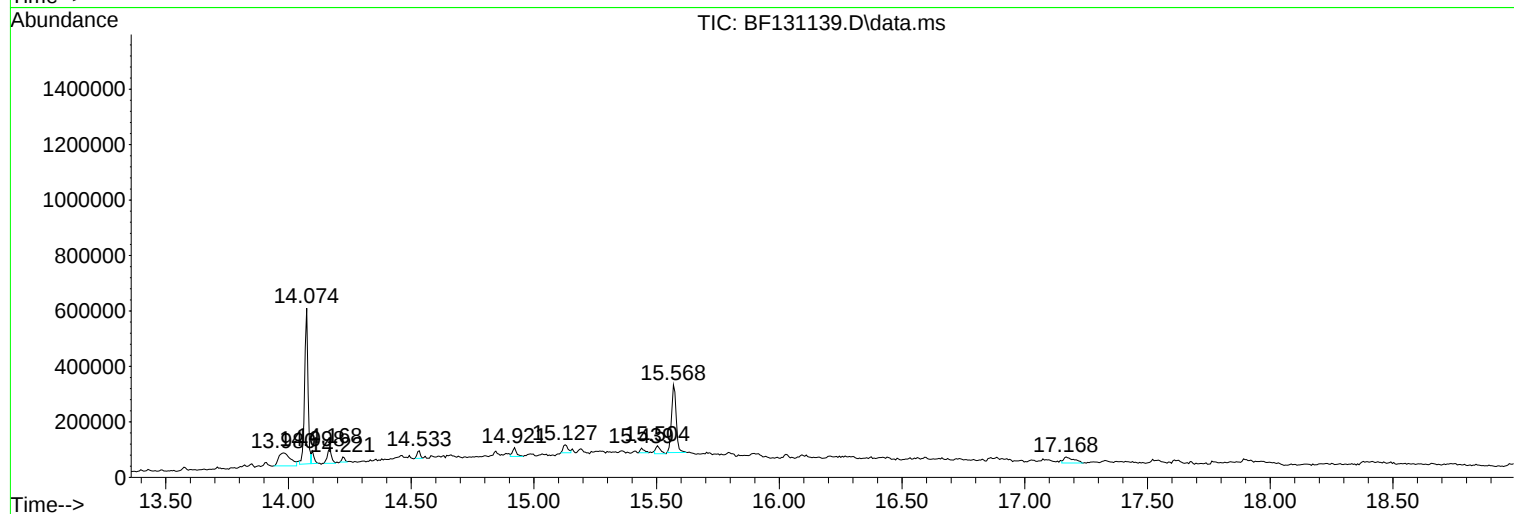
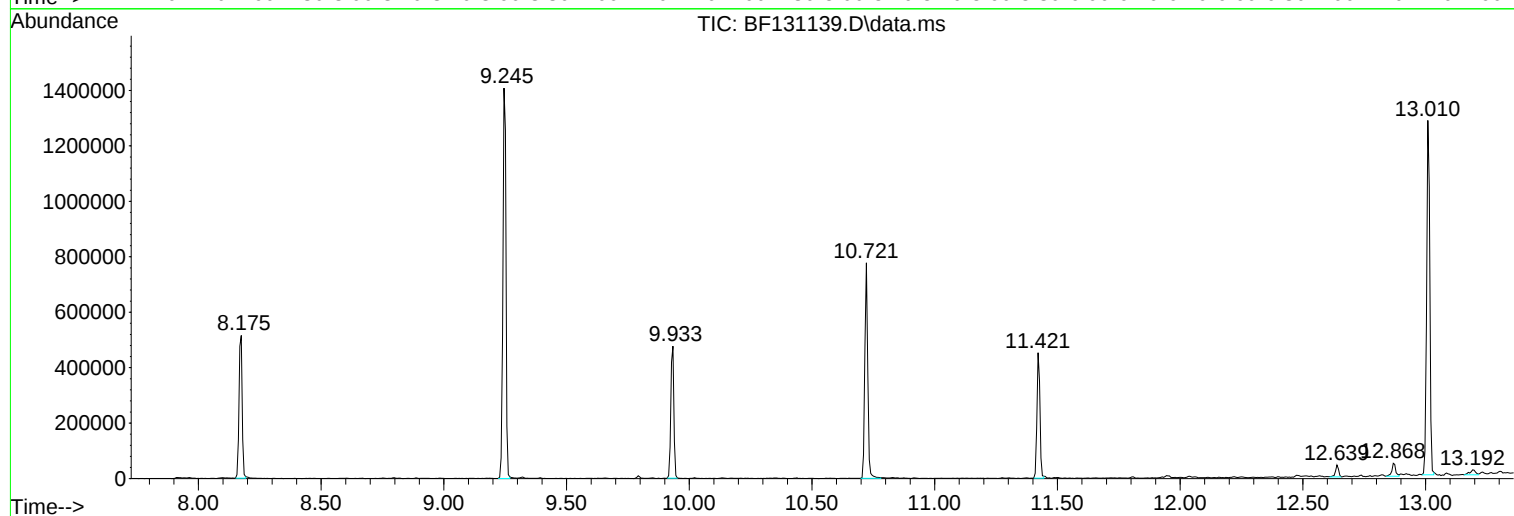
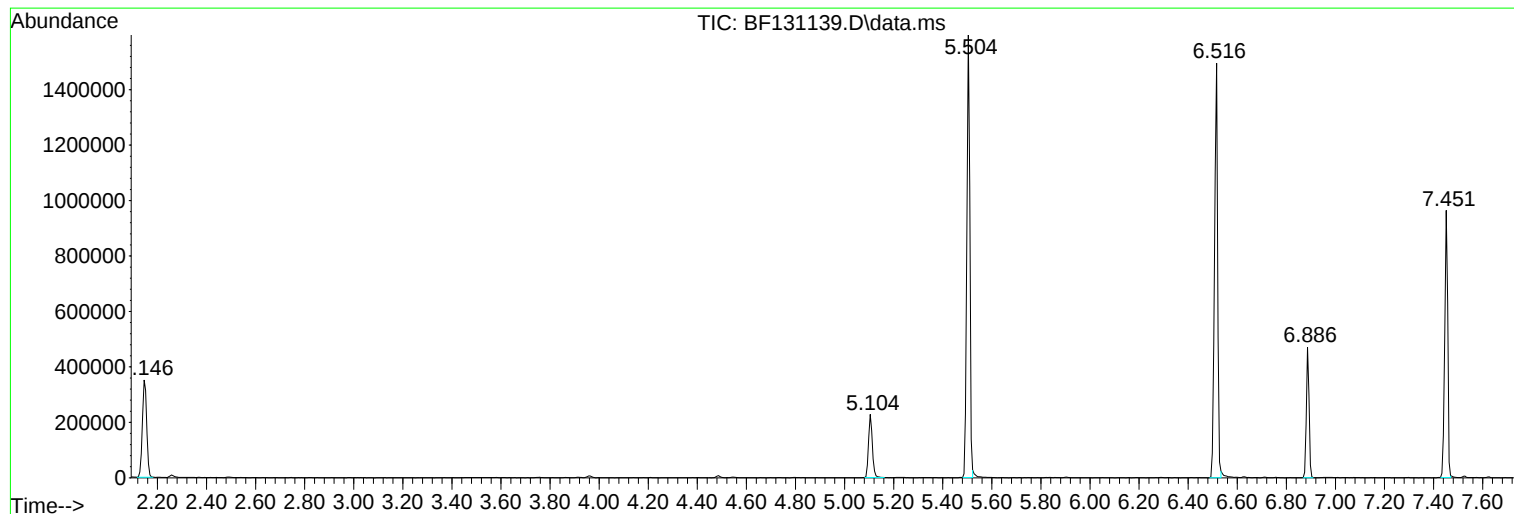
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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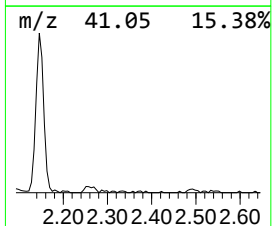
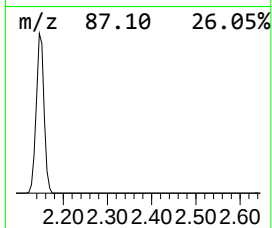
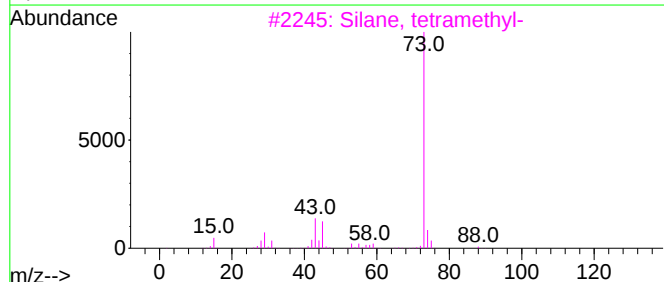
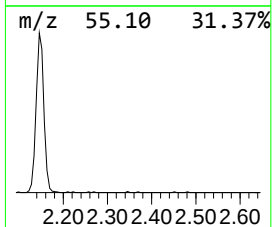
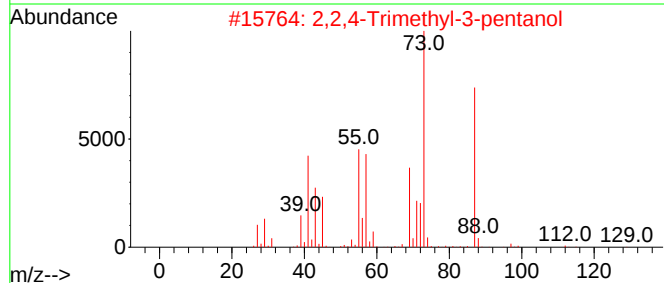
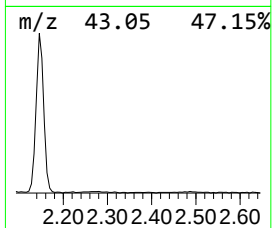
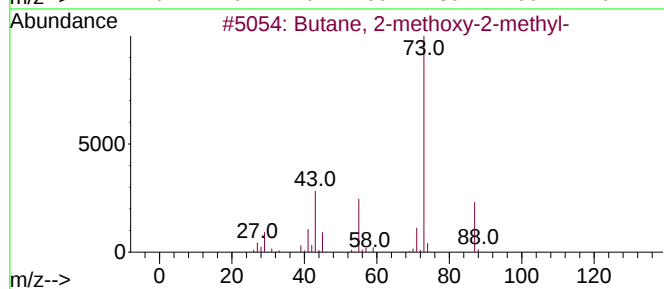
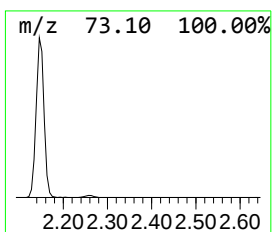
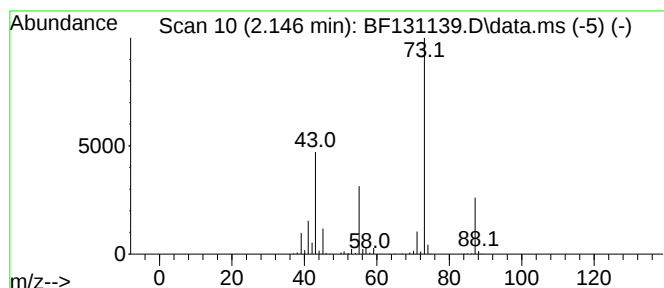
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	23.62 ng	428406	1,4-Dichlorobenzene-d4	6.886

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			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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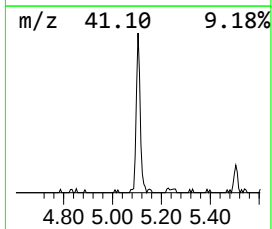
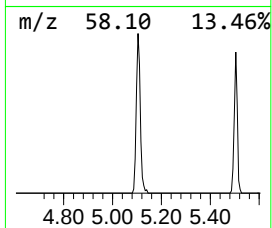
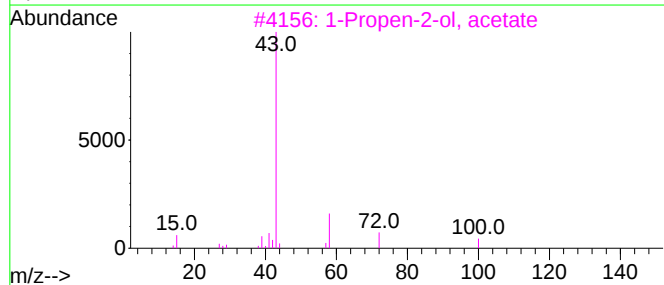
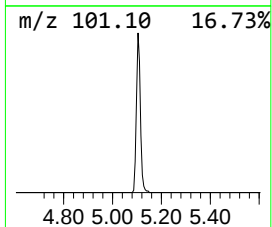
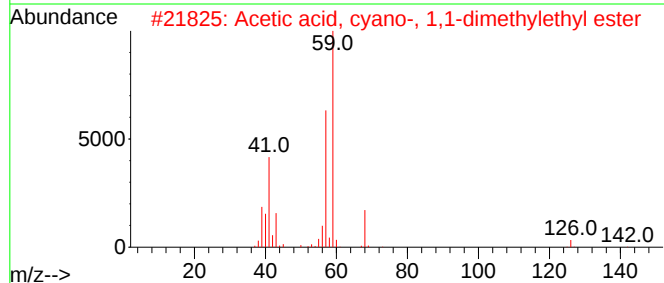
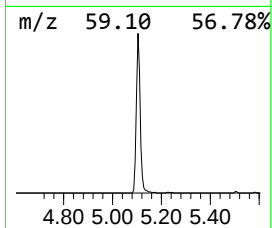
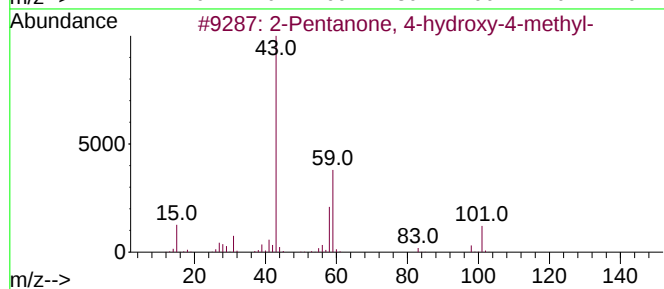
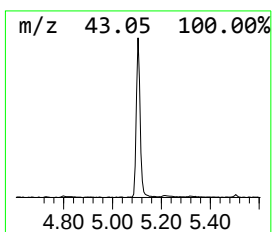
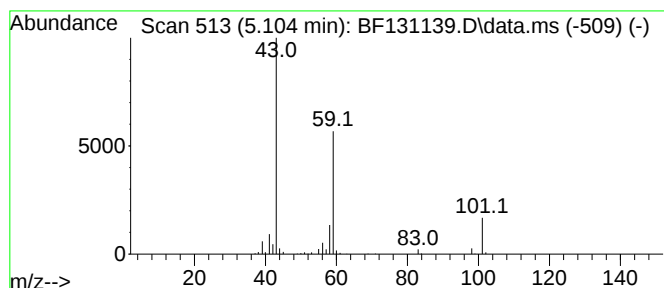
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	13.63 ng	247175	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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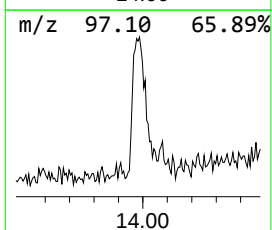
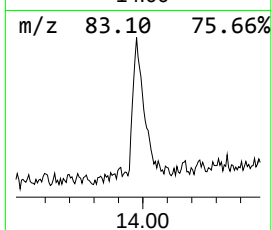
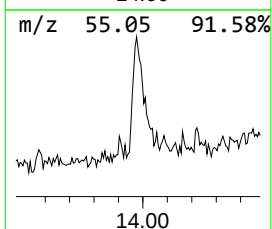
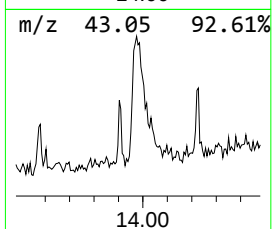
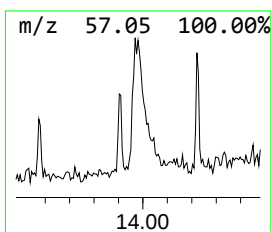
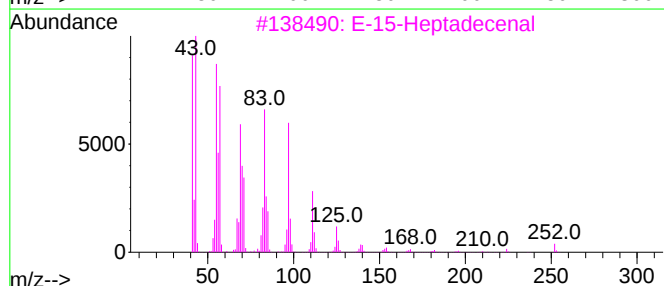
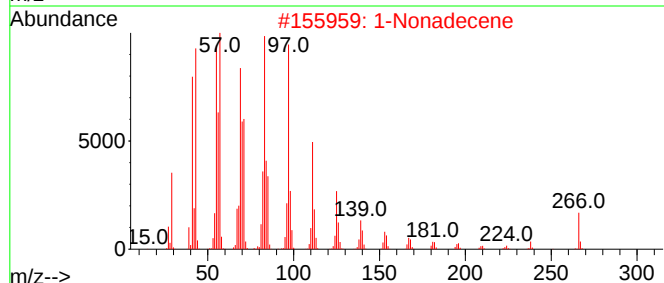
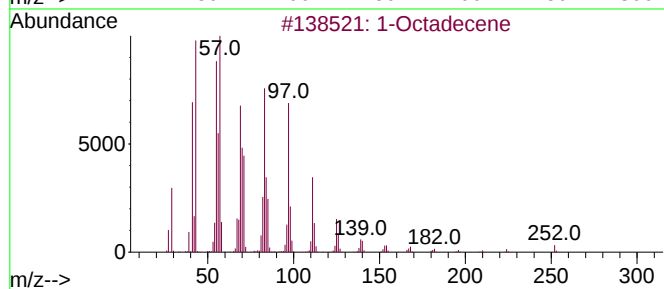
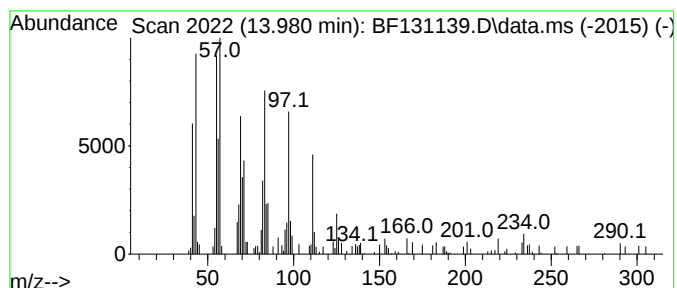
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Octadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	5.82 ng	156526	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecene	252	C18H36	000112-88-9	98
2			1-Nonadecene	266	C19H38	018435-45-5	97
3			E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5			1-Tetracosene	336	C24H48	010192-32-2	93



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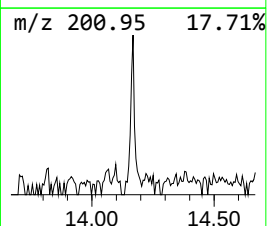
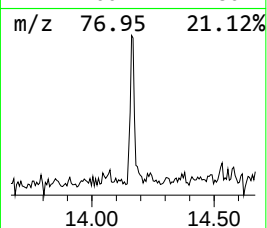
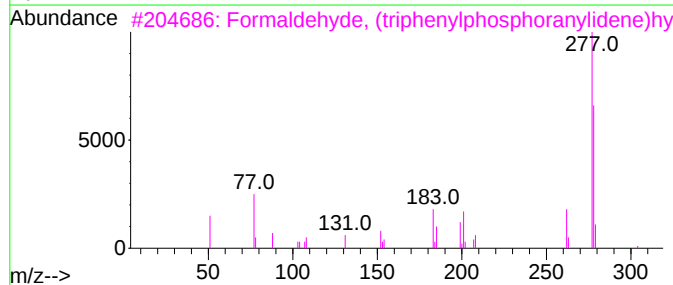
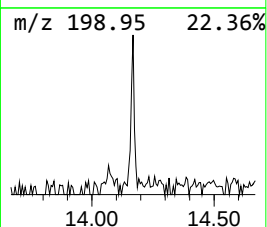
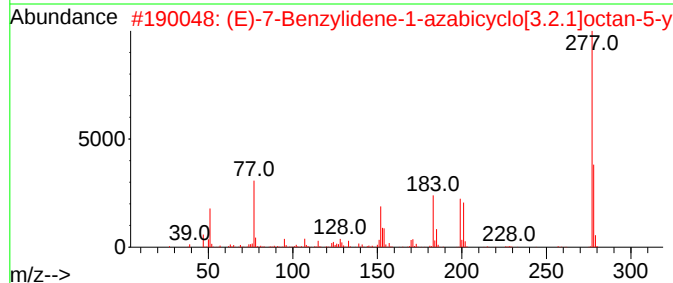
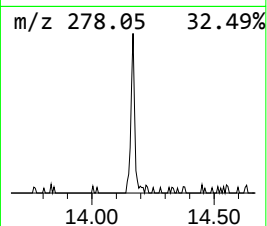
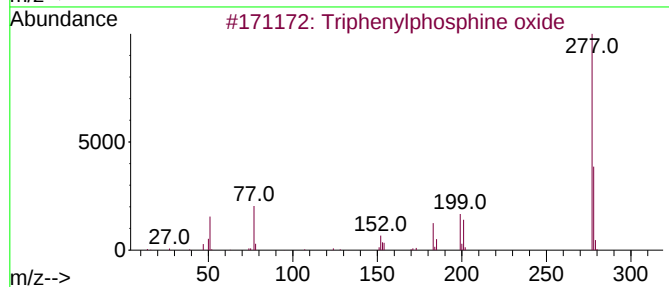
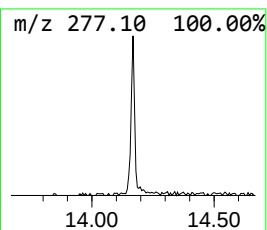
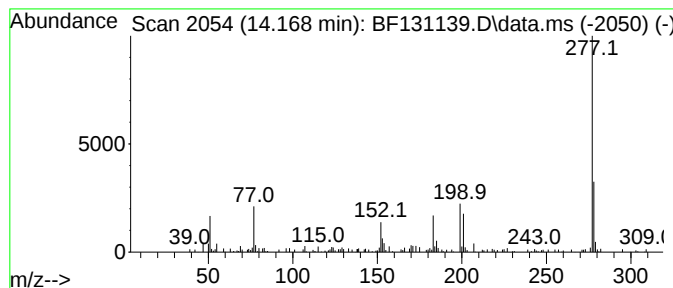
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.168	2.30 ng	61782	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	86
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	45
4			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	43
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	32



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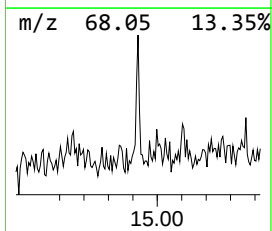
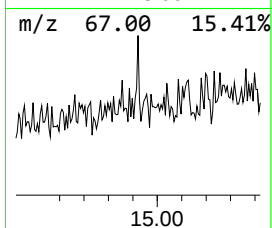
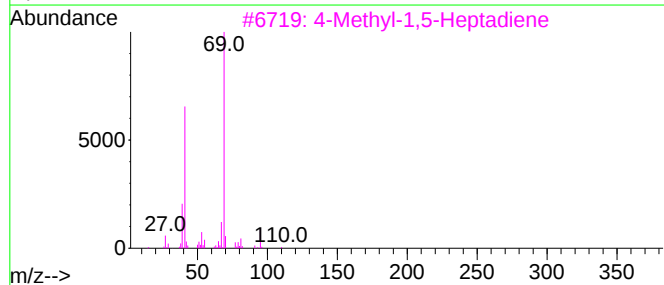
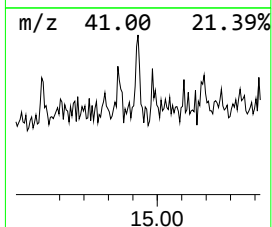
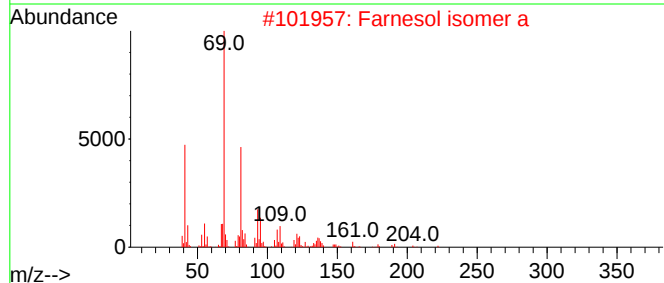
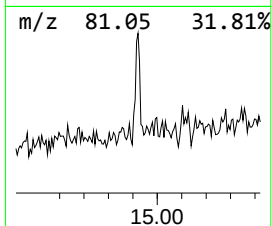
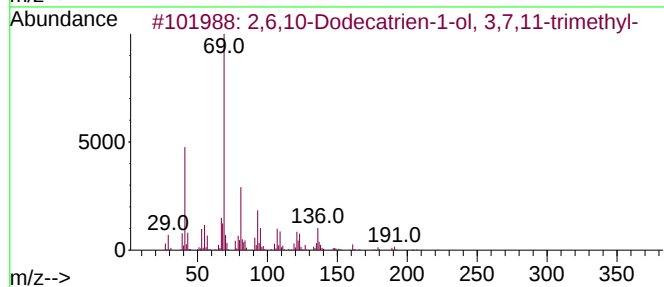
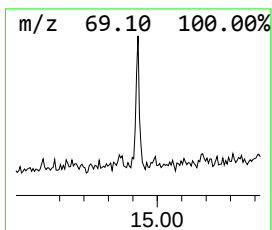
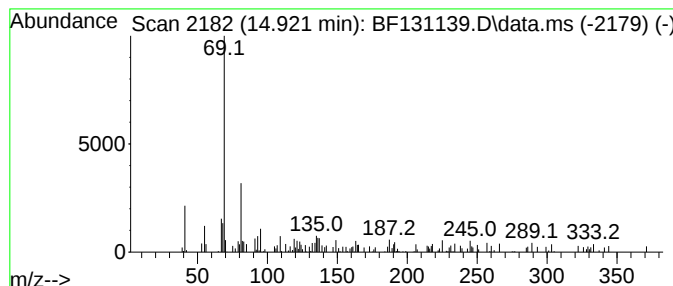
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Peak Number 5 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	2.16 ng	34750	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	62		
2	Farnesol isomer a	222	C15H26O	1000108-92-4	62		
3	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	53		
4	3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	53		
5	1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	50		



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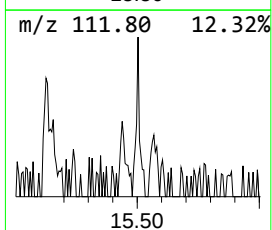
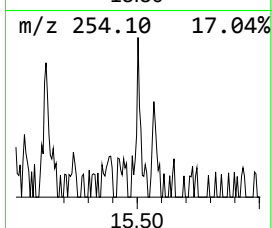
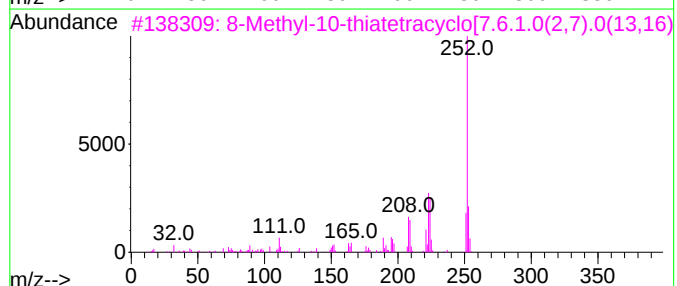
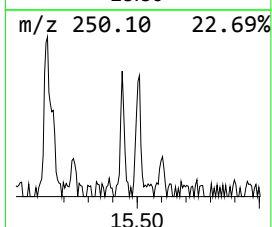
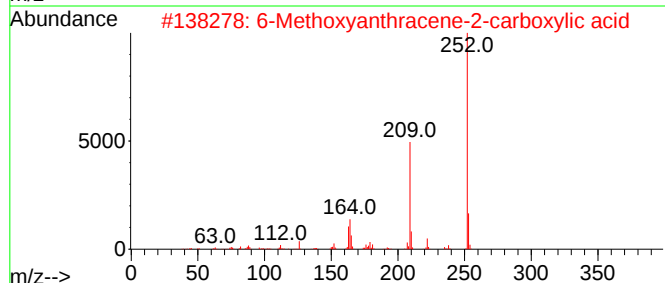
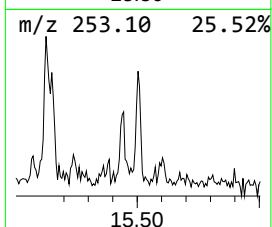
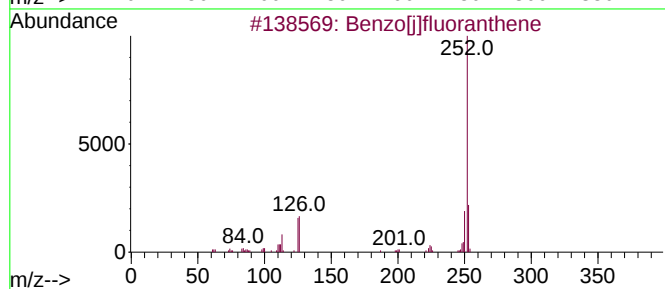
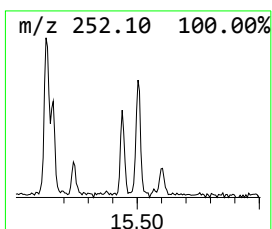
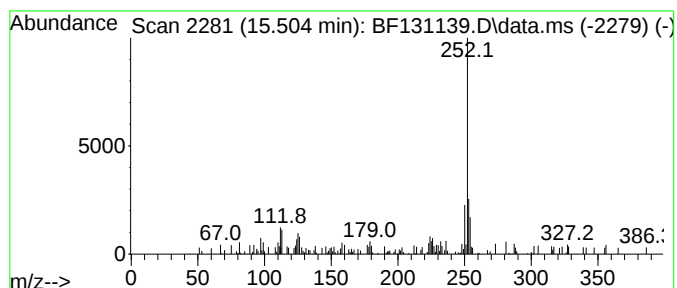
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[j]fluoranthene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.504	2.26 ng	36291	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[j]fluoranthene	252	C20H12	000205-82-3	52
2			6-Methoxyanthracene-2-carboxylic...	252	C16H12O3	240121-95-3	52
3			8-Methyl-10-thiatetracyclo[7.6.1...	252	C16H12O5	1000445-24-7	52
4			Perylene	252	C20H12	000198-55-0	52
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131139.D
Acq On : 10 Nov 2022 23:44
Operator : CG\JU
Sample : N5494-17
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20

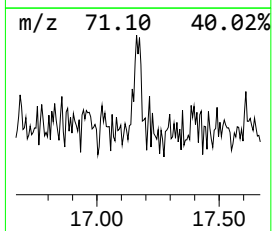
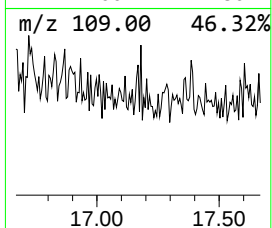
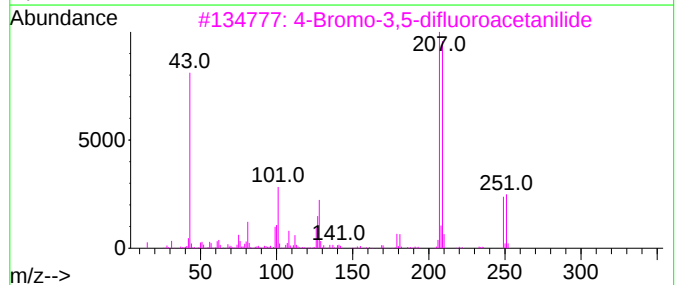
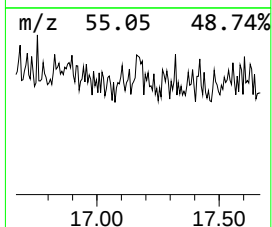
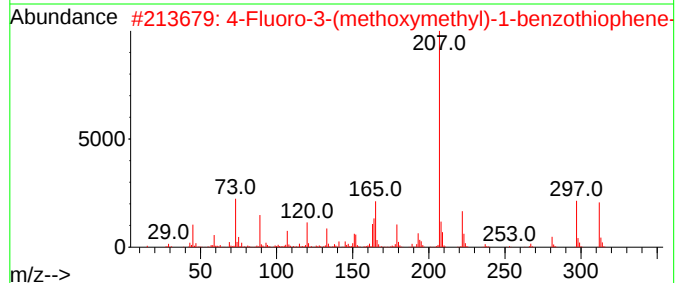
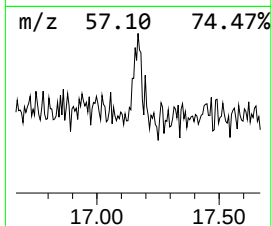
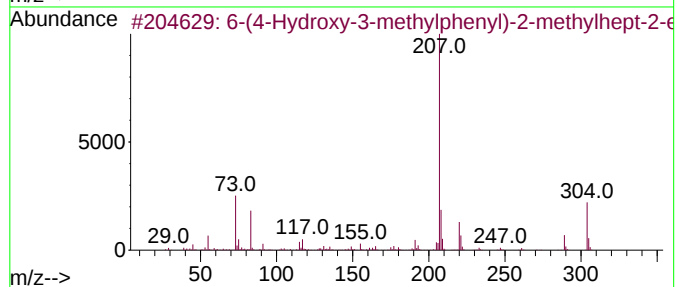
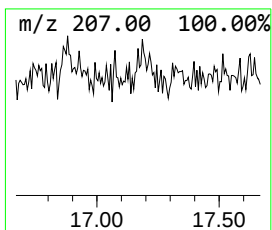
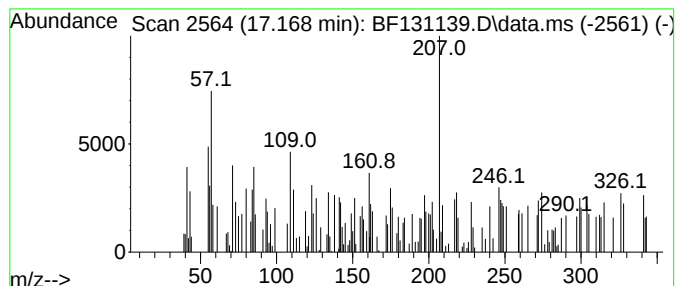
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.168 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.168	3.81 ng	61194	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-(4-Hydroxy-3-methylphenyl)-2-m...	304	C18H28O2Si	1000503-83-7	22		
2	4-Fluoro-3-(methoxymethyl)-1-ben...	312	C14H17F03SSi	1000502-78-0	20		
3	4-Bromo-3,5-difluoroacetanilide	249	C8H6BrF2NO	541539-64-4	18		
4	2-Bromo-4,6-difluoroaniline	207	C6H4BrF2N	000444-14-4	18		
5	Anthranilic acid, N-methyl-, but...	207	C12H17NO2	015236-34-7	18		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131139.D
Acq On : 10 Nov 2022 23:44
Operator : CG\JU
Sample : N5494-17
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	23.6	ng	428406	1	6.886	362730	20.0
2-Pentanone, 4-...	5.104	13.6	ng	247175	1	6.886	362730	20.0
1-Octadecene	13.980	5.8	ng	156526	5	14.074	538301	20.0
Triphenylphosph...	14.168	2.3	ng	61782	5	14.074	538301	20.0
2,6,10-Dodecatr...	14.921	2.2	ng	34750	6	15.568	321357	20.0
Benzo[j]fluoran...	15.504	2.3	ng	36291	6	15.568	321357	20.0
unknown17.168	17.168	3.8	ng	61194	6	15.568	321357	20.0