

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
 Data File : BF131018.D
 Acq On : 05 Nov 2022 14:15
 Operator : CG\JU
 Sample : N5335-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-1

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131018.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	10	18	25	rVB	1151605	1539205	54.86%	8.546%
2	5.122	512	516	524	rBV	133700	144218	5.14%	0.801%
3	5.516	579	583	587	rBV	1247695	1169056	41.67%	6.491%
4	6.522	750	754	767	rBV	792032	764228	27.24%	4.243%
5	6.904	815	819	822	rBV	520473	441399	15.73%	2.451%
6	6.957	825	828	836	rBV	77327	95492	3.40%	0.530%
7	7.469	910	915	918	rBV	1649633	1573951	56.10%	8.739%
8	8.087	1017	1020	1033	rBV	80215	145490	5.19%	0.808%
9	8.187	1033	1037	1040	rBV	708743	572791	20.42%	3.180%
10	8.634	1099	1113	1116	rBV	867214	2322745	82.79%	12.896%
11	9.263	1215	1220	1224	rBV	2733805	2805495	100.00%	15.576%
12	9.945	1332	1336	1340	rVB	769282	641322	22.86%	3.561%
13	10.363	1402	1407	1411	rVB	111606	89637	3.20%	0.498%
14	10.739	1466	1471	1474	rBV	1798327	1642227	58.54%	9.118%
15	11.439	1586	1590	1593	rBV	762189	611760	21.81%	3.396%
16	12.374	1744	1749	1759	rBV2	20104	39415	1.40%	0.219%
17	12.974	1848	1851	1856	rBV	66043	68746	2.45%	0.382%
18	13.033	1856	1861	1864	rVV	2473023	2311215	82.38%	12.832%
19	13.392	1917	1922	1928	rBV	21699	37389	1.33%	0.208%
20	13.974	2016	2021	2030	rBV4	32703	70937	2.53%	0.394%
21	14.086	2037	2040	2043	rVB	519401	413472	14.74%	2.296%
22	14.180	2052	2056	2062	rBV	75349	80790	2.88%	0.449%
23	14.292	2072	2075	2085	rBV2	19421	40224	1.43%	0.223%
24	15.586	2290	2295	2302	rVB	319223	390305	13.91%	2.167%

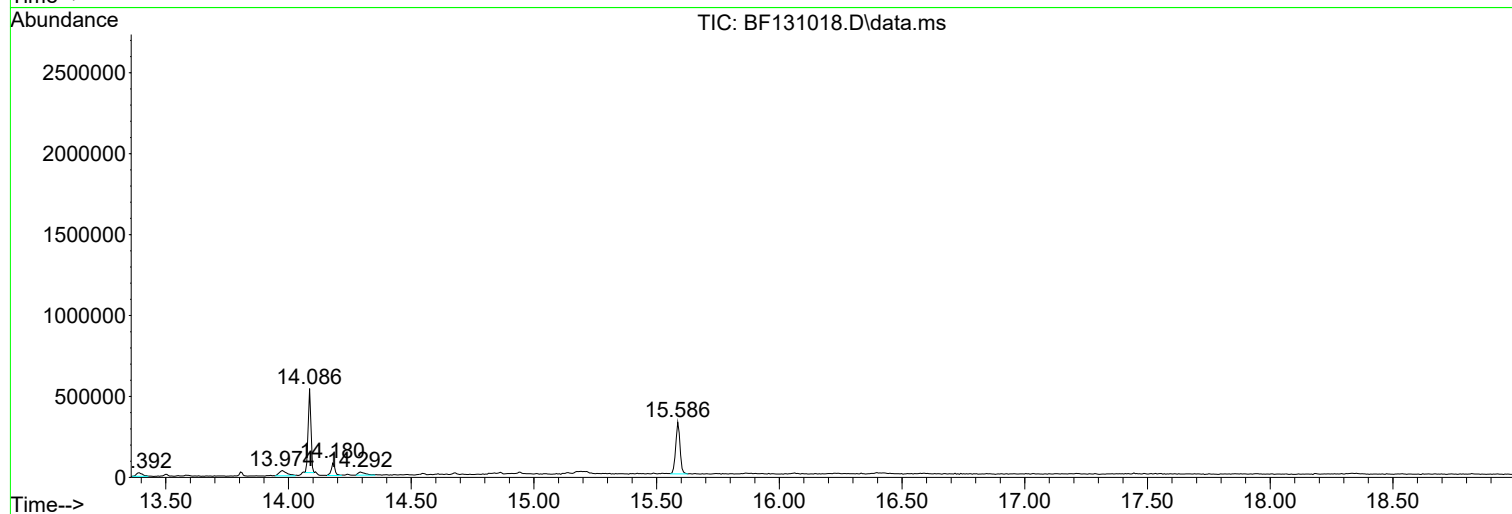
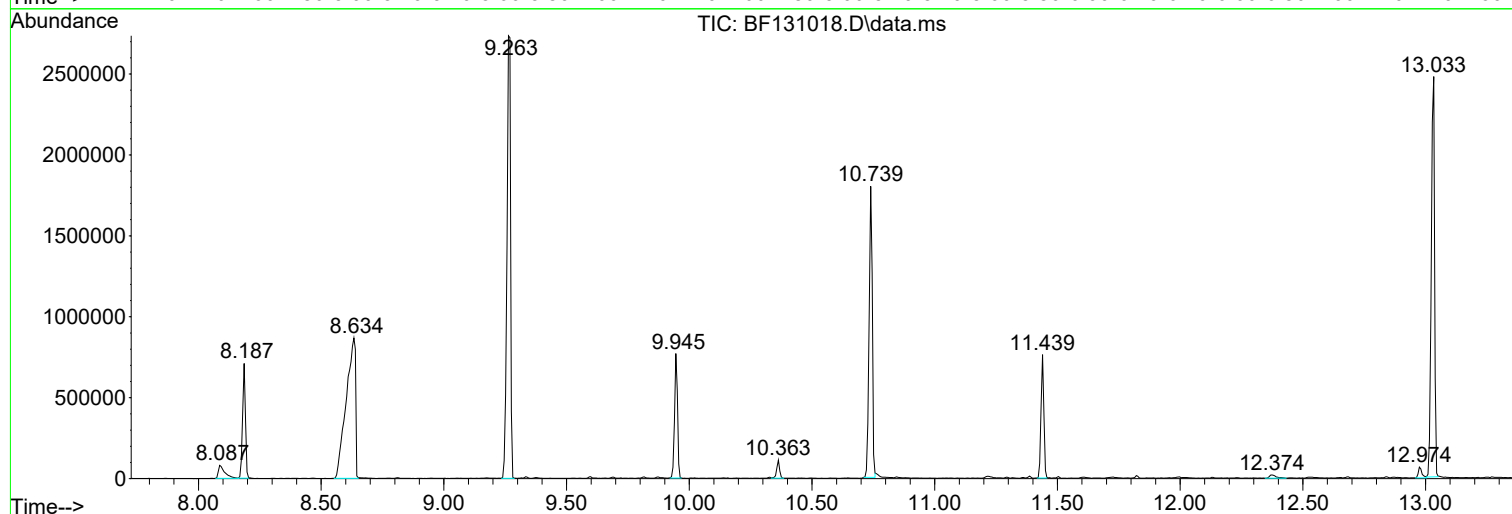
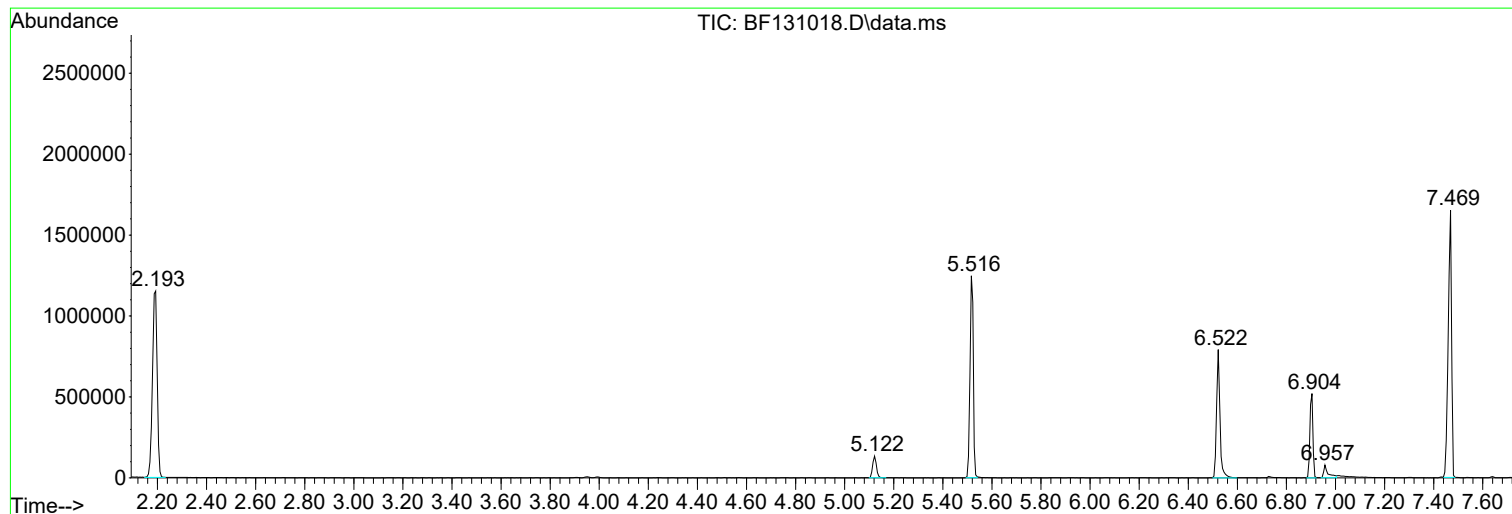
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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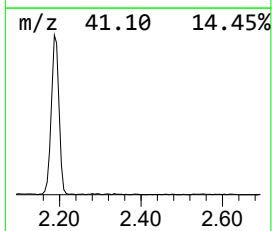
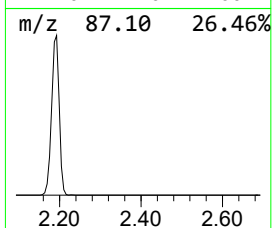
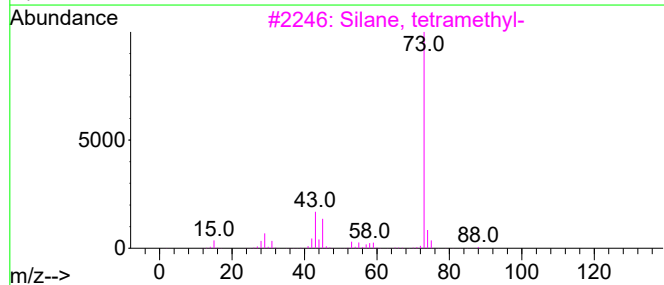
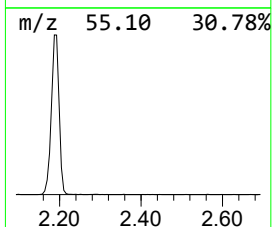
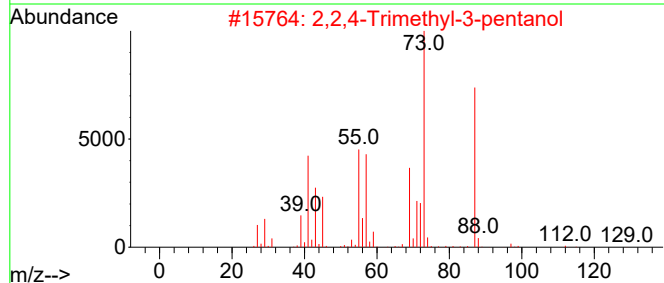
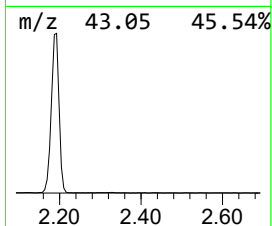
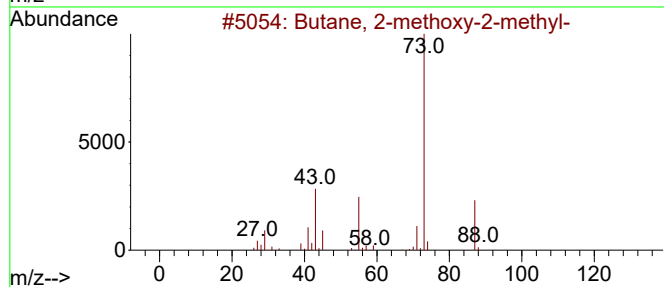
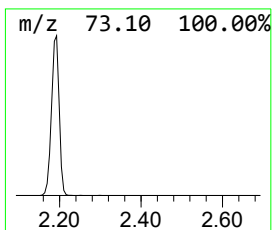
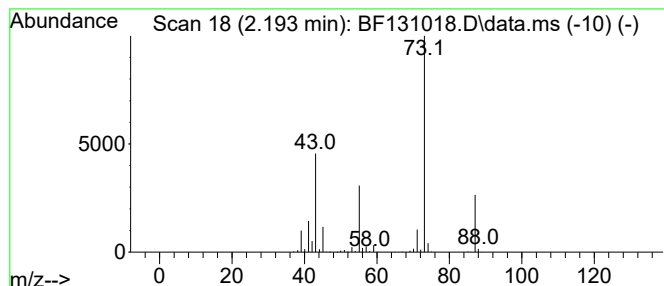
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	69.74 ng	1539210	1,4-Dichlorobenzene-d4	6.904

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	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
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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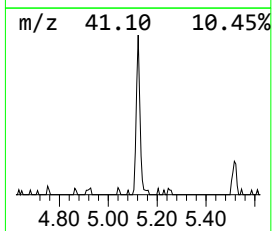
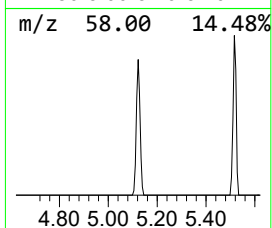
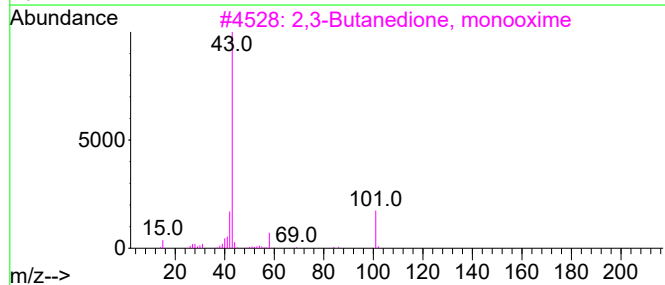
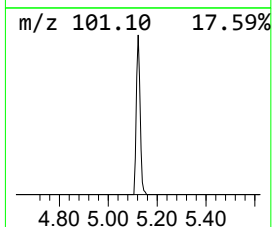
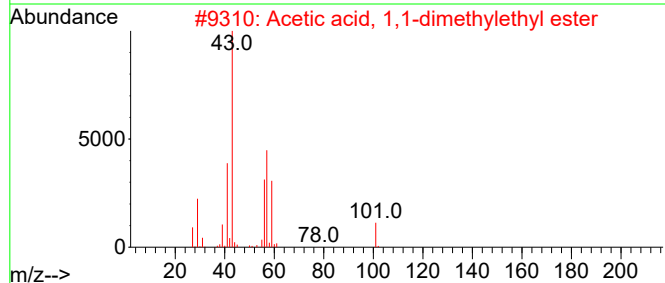
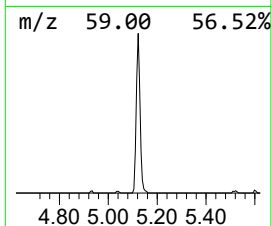
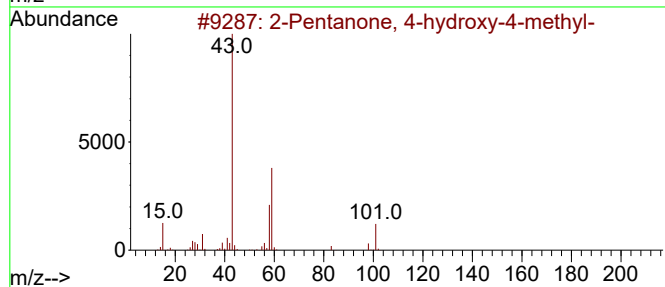
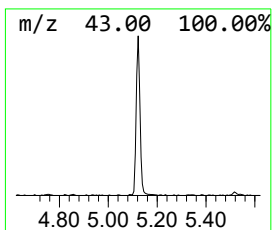
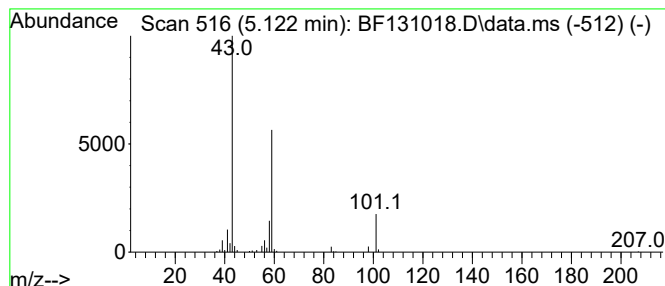
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	6.53 ng	144218	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25



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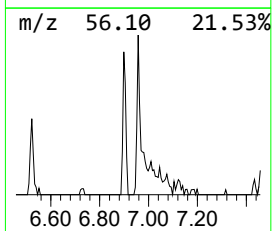
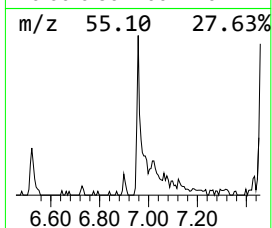
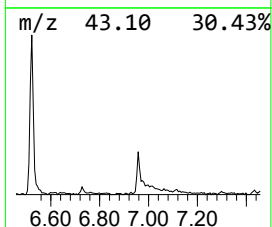
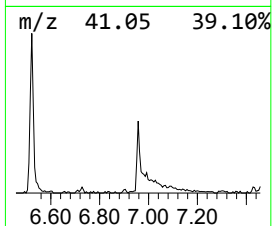
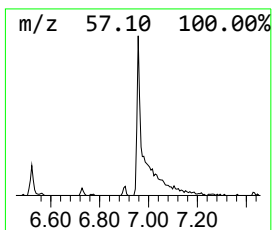
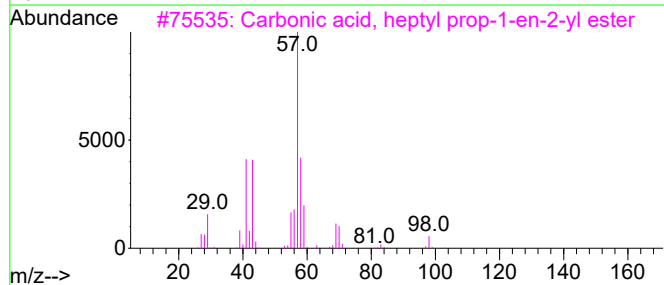
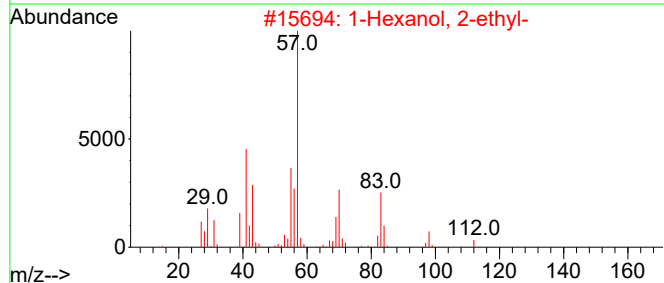
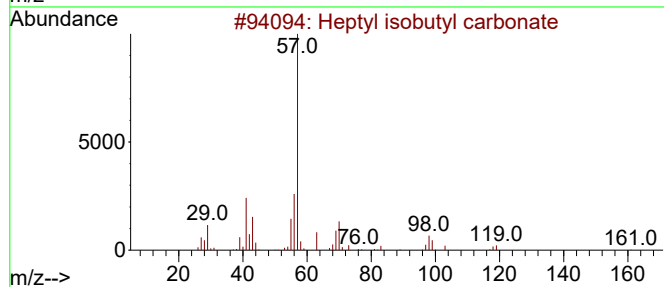
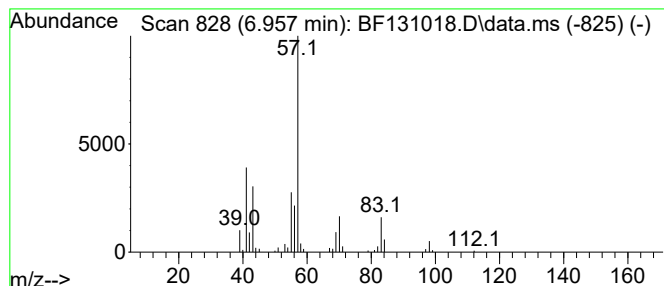
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Peak Number 3 Heptyl isobutyl carbonate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.957	4.33 ng	95492	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	64
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
3			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	53
4			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	50
5			Heptane, 3-ethyl-	128	C9H20	015869-80-4	50



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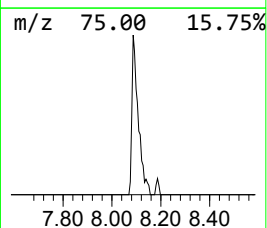
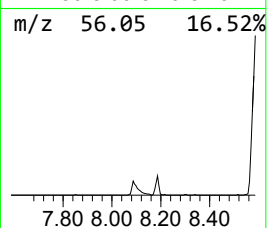
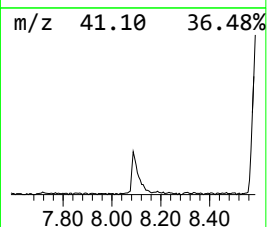
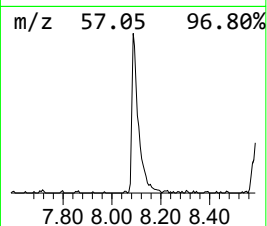
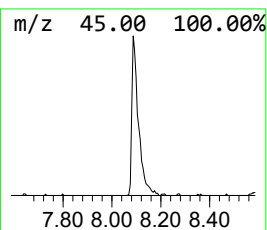
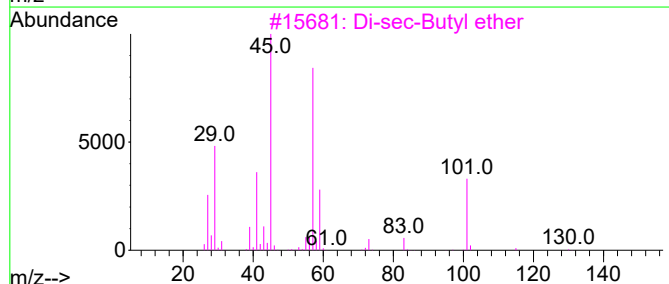
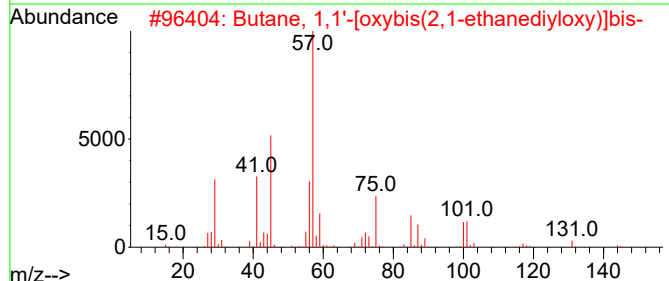
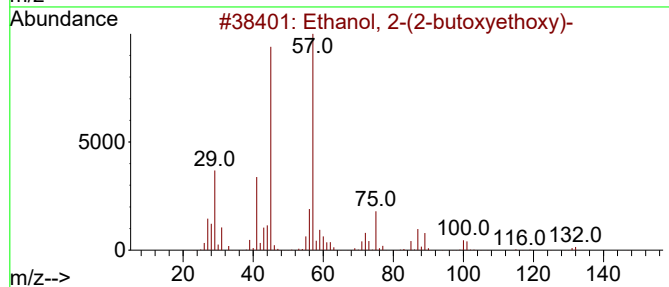
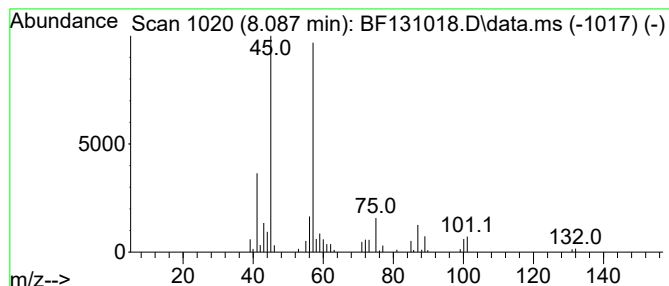
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.087	5.08 ng	145490	Naphthalene-d8	8.187

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	72
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53



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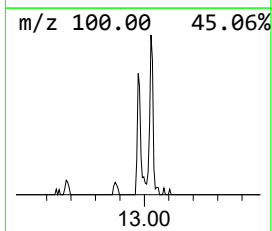
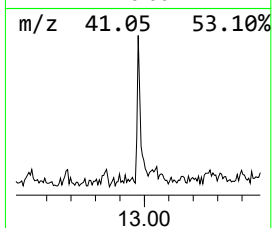
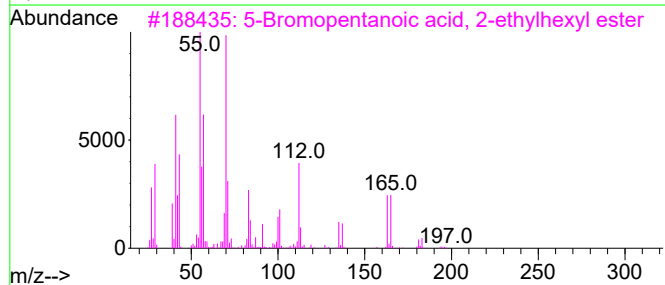
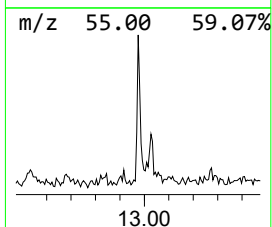
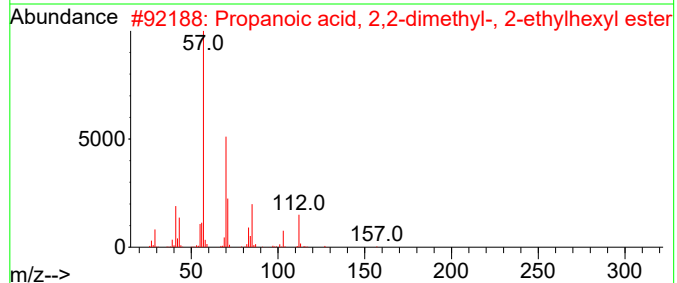
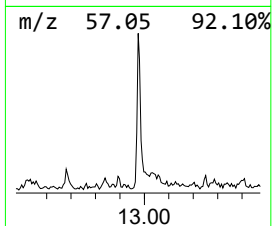
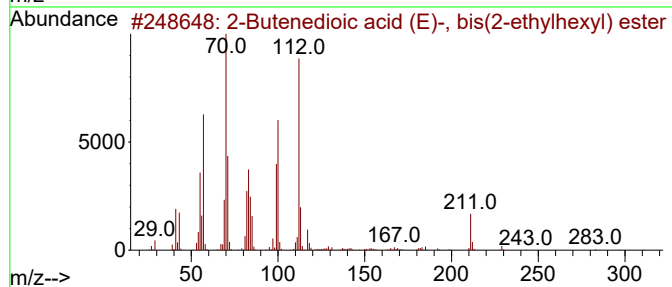
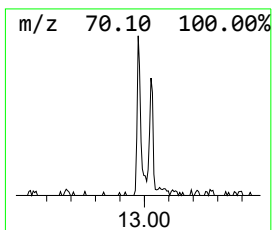
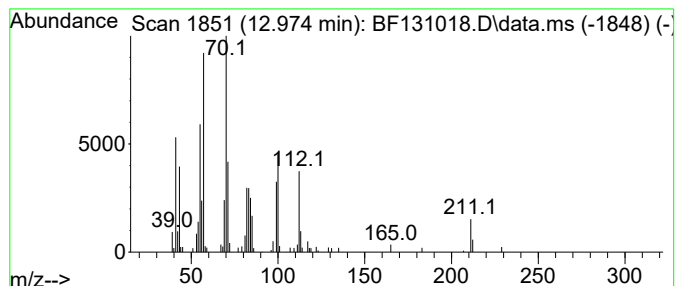
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Peak Number 5 2-Butenedioic acid (E)-, bi... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.974	3.33 ng	68746	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenedioic acid (E)-, bis(2-e...	340	C20H36O4	000141-02-6	90
2			Propanoic acid, 2,2-dimethyl-, 2...	214	C13H26O2	016387-18-1	47
3			5-Bromopentanoic acid, 2-ethylhe...	292	C13H25BrO2	1000293-55-4	43
4			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	43
5			Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	38



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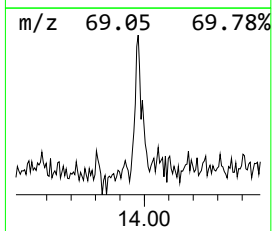
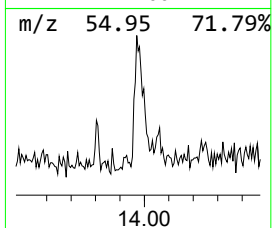
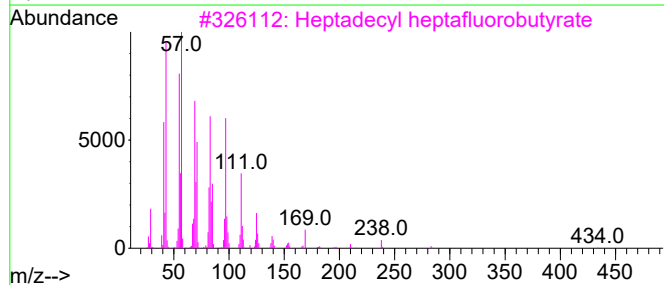
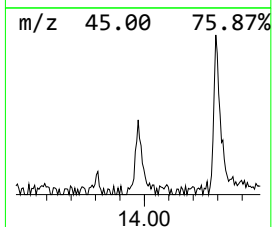
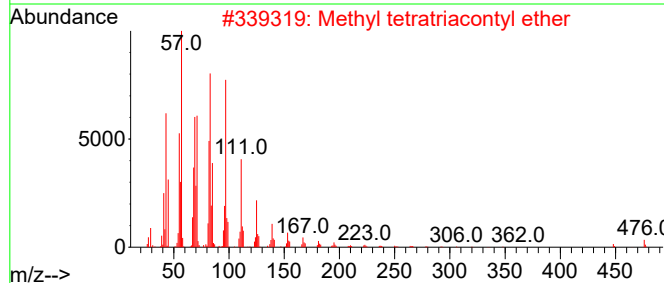
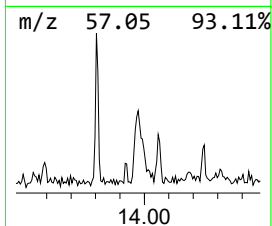
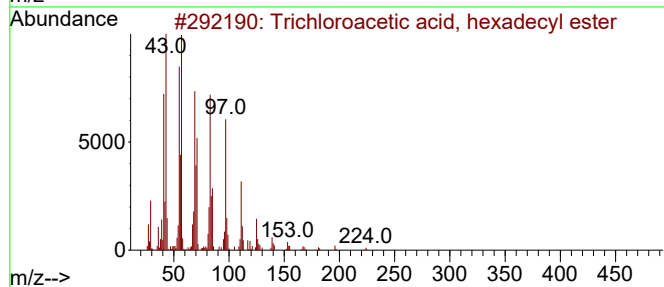
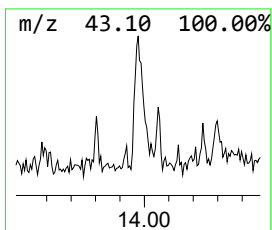
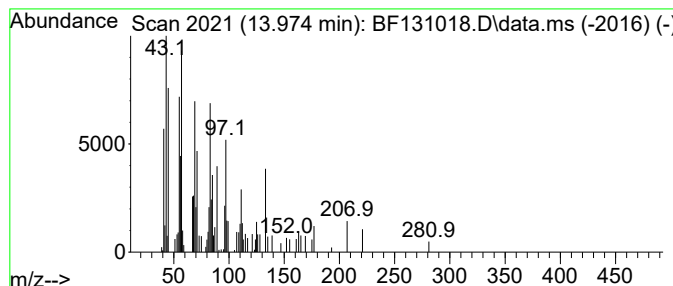
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	3.43 ng	70937	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64
2			Methyl tetratriacontyl ether	509	C35H72O	1000406-30-1	55
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	50
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	49
5			17-Pentatriacontene	491	C35H70	006971-40-0	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131018.D
Acq On : 05 Nov 2022 14:15
Operator : CG\JU
Sample : N5335-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

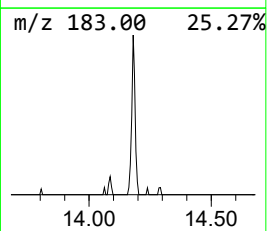
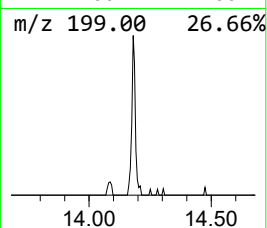
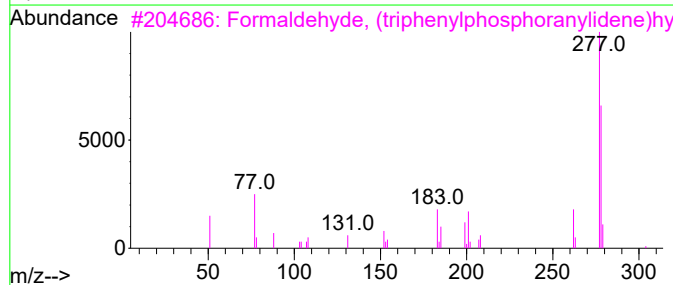
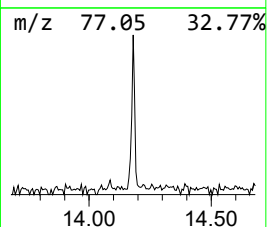
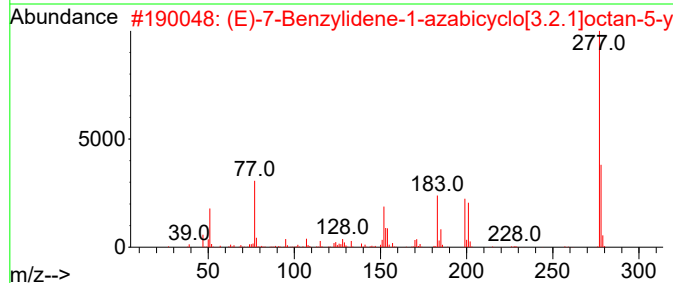
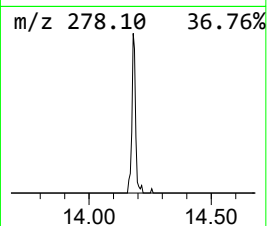
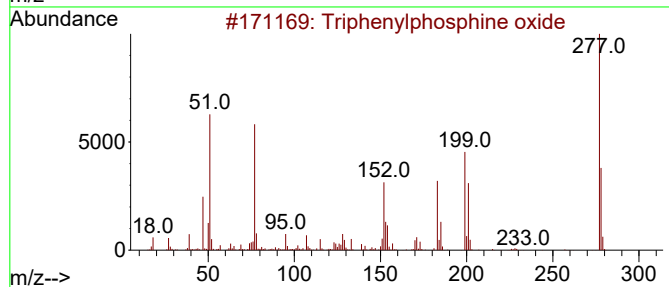
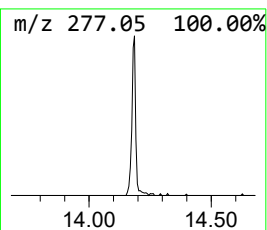
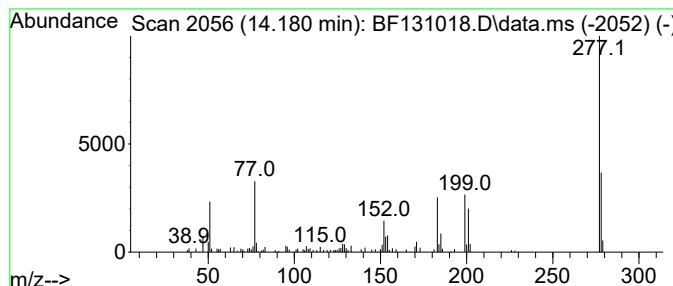
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.180	3.91 ng	80790	Chrysene-d12	14.086

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	87
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	25
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131018.D
Acq On : 05 Nov 2022 14:15
Operator : CG\JU
Sample : N5335-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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...	2.193	69.7	ng	1539210	1	6.904	441399	20.0
2-Pentanone, 4-...	5.122	6.5	ng	144218	1	6.904	441399	20.0
Heptyl isobutyl...	6.957	4.3	ng	95492	1	6.904	441399	20.0
Ethanol, 2-(2-b...	8.087	5.1	ng	145490	2	8.187	572791	20.0
2-Butenedioic a...	12.974	3.3	ng	68746	5	14.086	413472	20.0
Trichloroacetic...	13.974	3.4	ng	70937	5	14.086	413472	20.0
Triphenylphosph...	14.180	3.9	ng	80790	5	14.086	413472	20.0